乙二醇作为反应物的反应表19-9

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: -5312.08193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.91029 HOMO: -6.91169 LUMO: -0.53879 factor:1 | 1 (-1.46267) | -1 | -1 |
| G: -5312.08193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11578.02831 HOMO: -7.29809 LUMO: 2.83543 factor:1 | 1 (-1.58068) | 1 | -1 |
| G: -5312.08193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11578.37950 HOMO: -6.86543 LUMO: -0.70205 factor:1 | 1 (-1.93187) | -1 | -1 |
| G: -5312.08193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11578.22298 HOMO: -7.47769 LUMO: 0.31293 factor:1 | 1 (-1.77535) | -1 | -1 |
| G: -5312.08193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11578.33262 HOMO: -6.63141 LUMO: -0.55511 factor:1 | 1 (-1.88499) | -1 | -1 |
| G: -5312.08193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.01199 HOMO: -6.68856 LUMO: -0.30205 factor:1 | 1 (-0.56436) | -1 | -1 |
| G: -5312.08193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.90432 HOMO: -7.22190 LUMO: 0.53334 factor:1 | 1 (-0.45669) | -1 | -1 |
| G: -5312.08193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.92502 HOMO: -6.66407 LUMO: -0.27756 factor:1 | 1 (-0.47740) | -1 | -1 |
| G: -5312.08193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.15861 HOMO: -7.15659 LUMO: -0.70205 factor:1 | 1 (-0.71098) | -1 | -1 |
| G: -5312.08193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11578.59148 HOMO: -6.69400 LUMO: 1.67622 factor:1 | 1 (-2.14385) | -1 | -1 |
| G: -5312.08193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.94219 HOMO: -6.60420 LUMO: 2.16058 factor:1 | 1 (-1.49456) | -1 | -1 |
| G: -5312.08193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.91201 HOMO: -6.87087 LUMO: 1.88031 factor:1 | 1 (-1.46438) | -1 | -1 |
| G: -5312.08193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.96205 HOMO: -6.60965 LUMO: -0.19864 factor:1 | 1 (-1.51442) | -1 | -1 |
| G: -5312.08193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.99577 HOMO: -7.29265 LUMO: 0.52246 factor:1 | 1 (-0.54815) | -1 | -1 |
| G: -5312.08193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.90045 HOMO: -6.86543 LUMO: -0.59593 factor:1 | 1 (-0.45282) | -1 | -1 |
| G: -5312.08193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.05071 HOMO: -7.44504 LUMO: -1.01226 factor:1 | 1 (-0.60309) | -1 | -1 |
| G: -5312.08193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.38057 HOMO: -6.92530 LUMO: -0.75103 factor:1 | 1 (-0.93294) | -1 | -1 |
| G: -5312.08193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.16176 HOMO: -7.10489 LUMO: 2.20412 factor:1 | 1 (-0.71414) | 1 | 1 |
| G: -5312.08193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.94481 HOMO: -6.58788 LUMO: 1.73881 factor:1 | 1 (-0.49718) | -1 | -1 |
| G: -5312.08193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.86679 HOMO: -6.64502 LUMO: 1.70343 factor:1 | 1 (-0.41916) | -1 | -1 |
| G: -5312.08193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.16906 HOMO: -6.73754 LUMO: 1.60819 factor:1 | 1 (-0.72143) | -1 | -1 |
| G: -5312.08193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.93460 HOMO: -6.80829 LUMO: 2.45991 factor:1 | 1 (-0.48697) | -1 | -1 |
| G: -5312.08193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.21706 HOMO: -6.91713 LUMO: 2.43814 factor:1 | 1 (-0.76943) | -1 | -1 |
| G: -5312.08193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.88181 HOMO: -6.60692 LUMO: 1.93745 factor:1 | 1 (-0.43418) | -1 | -1 |
| G: -5312.08193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.90274 HOMO: -6.26134 LUMO: 1.46125 factor:1 | 1 (-0.45511) | -1 | -1 |
| G: -5312.08193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.03129 HOMO: -7.54028 LUMO: 0.25851 factor:1 | 1 (-0.58366) | -1 | -1 |
| G: -5312.08193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.05471 HOMO: -6.97700 LUMO: -0.73471 factor:1 | 1 (-0.60709) | -1 | -1 |
| G: -5312.08193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.27061 HOMO: -6.92258 LUMO: -0.70205 factor:1 | 1 (-0.82298) | -1 | -1 |
| G: -5312.08193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.14631 HOMO: -6.83550 LUMO: -0.56872 factor:1 | 1 (-0.69868) | -1 | -1 |
| G: -5312.08193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.00557 HOMO: -6.72121 LUMO: 1.89663 factor:1 | 1 (-0.55794) | -1 | -1 |
| G: -5312.08193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.11578 HOMO: -6.73482 LUMO: 1.89935 factor:1 | 1 (-0.66815) | -1 | -1 |
| G: -5312.08193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.31690 HOMO: -6.61781 LUMO: 1.86670 factor:1 | 1 (-0.86927) | -1 | -1 |
| G: -5312.08193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.00252 HOMO: -7.01782 LUMO: 2.26399 factor:1 | 1 (-0.55489) | -1 | -1 |
| G: -5312.08193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.12522 HOMO: -7.23551 LUMO: 2.09800 factor:1 | 1 (-0.67759) | 1 | 1 |
| G: -5312.08193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.01020 HOMO: -7.13483 LUMO: 2.17963 factor:1 | 1 (-0.56257) | 1 | 1 |
| G: -5312.08193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.08067 HOMO: -6.22869 LUMO: 2.01092 factor:1 | 1 (-0.63305) | -1 | -1 |
| G: -5312.08193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.06127 HOMO: -6.80285 LUMO: 2.14970 factor:1 | 1 (-0.61364) | -1 | -1 |
| G: -5312.08193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.15706 HOMO: -7.21102 LUMO: 2.33746 factor:1 | 1 (-0.70943) | 1 | 1 |
| G: -5312.08193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.65244 HOMO: -6.39740 LUMO: 2.59597 factor:1 | 1 (-1.20481) | -1 | -1 |
| G: -5312.08193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.76240 HOMO: -7.07768 LUMO: 2.48168 factor:1 | 1 (-1.31477) | 1 | 1 |
| G: -5312.08193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.95296 HOMO: -7.11306 LUMO: 0.90614 factor:1 | 1 (-1.50533) | -1 | -1 |
| G: -5312.08193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.53309 HOMO: -6.61781 LUMO: -2.46263 factor:1 | 1 (-1.08546) | -1 | -1 |
| G: -5312.08193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.78809 HOMO: -6.96611 LUMO: 0.90614 factor:1 | 1 (-1.34046) | -1 | -1 |
| G: -5312.08193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.64134 HOMO: -6.86271 LUMO: -1.14832 factor:1 | 1 (-1.19371) | -1 | -1 |
| G: -5312.08193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11578.02616 HOMO: -6.72665 LUMO: 0.96873 factor:1 | 1 (-1.57853) | -1 | -1 |
| G: -5312.08193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.81554 HOMO: -7.14571 LUMO: 1.05036 factor:1 | 1 (-1.36792) | -1 | -1 |
| G: -5312.08193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.89647 HOMO: -7.14299 LUMO: 0.98777 factor:1 | 1 (-1.44884) | -1 | -1 |
| G: -5312.08193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.96118 HOMO: -6.99333 LUMO: 1.05852 factor:1 | 1 (-1.51355) | -1 | -1 |
| G: -5312.08193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.97621 HOMO: -6.78924 LUMO: -1.49935 factor:1 | 1 (-0.52858) | -1 | -1 |
| G: -5312.08193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.02353 HOMO: -7.13755 LUMO: 0.94151 factor:1 | 1 (-0.57590) | -1 | -1 |
| G: -5312.08193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.14419 HOMO: -6.72938 LUMO: -0.35375 factor:1 | 1 (-0.69656) | -1 | -1 |
| G: -5312.08193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.08429 HOMO: -6.99061 LUMO: 0.82450 factor:1 | 1 (-0.63666) | -1 | -1 |
| G: -5312.08193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.99433 HOMO: -6.75114 LUMO: -0.68028 factor:1 | 1 (-0.54670) | -1 | -1 |
| G: -5312.08193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.78886 HOMO: -6.40556 LUMO: -0.42722 factor:1 | 1 (-0.34123) | -1 | -1 |
| G: -5312.08193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.83689 HOMO: -7.18653 LUMO: 0.42178 factor:1 | 1 (-0.38926) | -1 | -1 |
| G: -5312.08193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.91945 HOMO: -6.63958 LUMO: -0.71294 factor:1 | 1 (-0.47182) | -1 | -1 |
| G: -5312.08193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.97485 HOMO: -6.63958 LUMO: -0.71022 factor:1 | 1 (-0.52722) | -1 | -1 |
| G: -5312.08193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.14516 HOMO: -6.69672 LUMO: -0.72654 factor:1 | 1 (-0.69754) | -1 | -1 |
| G: -5312.08193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.85101 HOMO: -6.56883 LUMO: -0.80274 factor:1 | 1 (-0.40338) | -1 | -1 |
| G: -5312.08193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.75041 HOMO: -6.68584 LUMO: -0.56872 factor:1 | 1 (-0.30278) | -1 | -1 |
| G: -5312.08193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.88045 HOMO: -6.59060 LUMO: -0.35647 factor:1 | 1 (-0.43282) | -1 | -1 |
| G: -5312.08193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.78189 HOMO: -6.72121 LUMO: -0.71838 factor:1 | 1 (-0.33426) | -1 | -1 |
| G: -5312.08193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.06329 HOMO: -6.57971 LUMO: -0.61498 factor:1 | 1 (-0.61566) | -1 | -1 |
| G: -5312.08193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.90037 HOMO: -7.07496 LUMO: 0.50613 factor:1 | 1 (-0.45274) | -1 | -1 |
| G: -5312.08193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.05787 HOMO: -7.14027 LUMO: 0.43266 factor:1 | 1 (-0.61024) | -1 | -1 |
| G: -5312.08193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11578.95440 HOMO: -6.43277 LUMO: -0.44082 factor:1 | 1 (-2.50677) | -1 | -1 |
| G: -5312.08193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11578.00401 HOMO: -6.79468 LUMO: 0.07619 factor:1 | 1 (-1.55638) | -1 | -1 |
| G: -5312.08193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11578.22633 HOMO: -6.81917 LUMO: -2.57148 factor:1 | 1 (-1.77870) | -1 | -1 |
| G: -5312.08193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11578.35074 HOMO: -6.71849 LUMO: 1.30615 factor:1 | 1 (-1.90311) | -1 | -1 |
| G: -5312.08193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.72037 HOMO: -6.85455 LUMO: -0.63675 factor:1 | 1 (-0.27274) | -1 | -1 |
| G: -5312.08193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.85237 HOMO: -6.73210 LUMO: -1.03131 factor:1 | 1 (-0.40474) | -1 | -1 |
| G: -5312.08193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.97158 HOMO: -6.83550 LUMO: -0.58777 factor:1 | 1 (-0.52396) | -1 | -1 |
| G: -5312.08193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.81248 HOMO: -6.53073 LUMO: -0.74287 factor:1 | 1 (-0.36485) | -1 | -1 |
| G: -5312.08193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.69759 HOMO: -7.18381 LUMO: -0.92791 factor:1 | 1 (-0.24996) | -1 | -1 |
| G: -5312.08193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11578.44543 HOMO: -6.49264 LUMO: -0.44627 factor:1 | 1 (-1.99781) | -1 | -1 |
| G: -5312.08193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.65519 HOMO: -7.32803 LUMO: 0.41361 factor:1 | 1 (-1.20756) | -1 | -1 |
| G: -5312.08193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.75337 HOMO: -6.53073 LUMO: -0.52790 factor:1 | 1 (-1.30574) | -1 | -1 |
| G: -5312.08193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.83933 HOMO: -6.54978 LUMO: -0.53062 factor:1 | 1 (-1.39170) | -1 | -1 |
| G: -5312.08193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.96779 HOMO: -6.56611 LUMO: -0.37824 factor:1 | 1 (-1.52016) | -1 | -1 |
| G: -5312.08193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.95855 HOMO: -6.57155 LUMO: -0.64219 factor:1 | 1 (-0.51092) | -1 | -1 |
| G: -5312.08193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.21649 HOMO: -7.08040 LUMO: 0.45715 factor:1 | 1 (-0.76886) | -1 | -1 |
| G: -5312.08193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.91822 HOMO: -6.66679 LUMO: -0.75376 factor:1 | 1 (-0.47059) | -1 | -1 |
| G: -5312.08193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.98994 HOMO: -6.83550 LUMO: -0.99322 factor:1 | 1 (-1.54231) | -1 | -1 |
| G: -5312.08193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.99277 HOMO: -6.53345 LUMO: -0.29660 factor:1 | 1 (-1.54514) | -1 | -1 |
| G: -5312.08193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.87527 HOMO: -6.65046 LUMO: 2.40549 factor:1 | 1 (-1.42765) | -1 | -1 |
| G: -5312.08193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.86178 HOMO: -6.98788 LUMO: 2.01092 factor:1 | 1 (-1.41415) | -1 | -1 |
| G: -5312.08193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.93106 HOMO: -6.61781 LUMO: 1.92384 factor:1 | 1 (-1.48343) | -1 | -1 |
| G: -5312.08193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11578.52731 HOMO: -6.61237 LUMO: 2.06807 factor:1 | 1 (-2.07968) | -1 | -1 |
| G: -5312.08193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.20008 HOMO: -6.59060 LUMO: 1.95106 factor:1 | 1 (-0.75245) | -1 | -1 |
| G: -5312.08193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11578.21245 HOMO: -6.48175 LUMO: 1.72248 factor:1 | 1 (-1.76482) | -1 | -1 |
| G: -5312.08193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11578.08701 HOMO: -6.84911 LUMO: 2.03541 factor:1 | 1 (-1.63938) | -1 | -1 |
| G: -5312.08193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.99424 HOMO: -6.50624 LUMO: 2.17147 factor:1 | 1 (-1.54661) | -1 | -1 |
| G: -5312.08193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.67342 HOMO: -6.68312 LUMO: 2.08439 factor:1 | 1 (-1.22579) | -1 | -1 |
| G: -5312.08193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.91821 HOMO: -6.96067 LUMO: 1.98099 factor:1 | 1 (-1.47058) | -1 | -1 |
| G: -5312.08193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11578.06709 HOMO: -6.93618 LUMO: 1.85854 factor:1 | 1 (-1.61946) | -1 | -1 |
| G: -5312.08193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.82091 HOMO: -6.71305 LUMO: -0.61226 factor:1 | 1 (-1.37328) | -1 | -1 |
| G: -5312.08193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.66515 HOMO: -7.06408 LUMO: 0.80001 factor:1 | 1 (-1.21752) | -1 | -1 |
| G: -5312.08193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.37486 HOMO: -6.52257 LUMO: 0.99049 factor:1 | 1 (-0.92723) | -1 | -1 |
| G: -5312.08193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.47339 HOMO: -6.84638 LUMO: 1.10750 factor:1 | 1 (-1.02576) | -1 | -1 |
| G: -5312.08193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.45910 HOMO: -6.85455 LUMO: 0.84900 factor:1 | 1 (-1.01147) | -1 | -1 |
| G: -5312.08193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.26756 HOMO: -6.60148 LUMO: -0.78369 factor:1 | 1 (-0.81993) | -1 | -1 |
| G: -5312.08193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.88371 HOMO: -6.86543 LUMO: -0.93063 factor:1 | 1 (-1.43608) | -1 | -1 |
| G: -5312.08193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.62332 HOMO: -6.70489 LUMO: -0.72382 factor:1 | 1 (-1.17570) | -1 | -1 |
| G: -5312.08193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.62354 HOMO: -6.59060 LUMO: 0.31293 factor:1 | 1 (-1.17591) | -1 | -1 |
| G: -5312.08193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.48607 HOMO: -6.52257 LUMO: -0.48708 factor:1 | 1 (-1.03844) | -1 | -1 |
| G: -5312.08193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.54626 HOMO: -6.54706 LUMO: -0.48164 factor:1 | 1 (-1.09863) | -1 | -1 |
| G: -5312.08193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.46640 HOMO: -7.32803 LUMO: 0.08436 factor:1 | 1 (-1.01877) | -1 | -1 |
| G: -5312.08193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.40193 HOMO: -6.77291 LUMO: -0.66940 factor:1 | 1 (-0.95430) | -1 | -1 |
| G: -5312.08193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.17673 HOMO: -6.68312 LUMO: -0.53062 factor:1 | 1 (-0.72910) | -1 | -1 |
| G: -5312.08193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.32386 HOMO: -7.07768 LUMO: 0.45987 factor:1 | 1 (-0.87623) | -1 | -1 |
| G: -5312.08193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.29080 HOMO: -6.50352 LUMO: -0.63675 factor:1 | 1 (-0.84317) | -1 | -1 |
| G: -5312.08193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.73803 HOMO: -6.48992 LUMO: -0.60681 factor:1 | 1 (-0.29040) | -1 | -1 |
| G: -5312.08193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.10696 HOMO: -6.65318 LUMO: -0.72382 factor:1 | 1 (-0.65933) | -1 | -1 |
| G: -5312.08193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.27080 HOMO: -6.54706 LUMO: 0.24218 factor:1 | 1 (-0.82317) | -1 | -1 |
| G: -5312.08193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.31456 HOMO: -6.63958 LUMO: 0.57416 factor:1 | 1 (-0.86693) | -1 | -1 |
| G: -5312.08193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.44906 HOMO: -6.37563 LUMO: -0.48164 factor:1 | 1 (-1.00143) | -1 | -1 |
| G: -5312.08193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.46435 HOMO: -6.64774 LUMO: -0.71838 factor:1 | 1 (-1.01673) | -1 | -1 |
| G: -5312.08193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.85116 HOMO: -7.17020 LUMO: 0.45987 factor:1 | 1 (-1.40354) | -1 | -1 |
| G: -5312.08193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11578.06088 HOMO: -6.86543 LUMO: -1.05036 factor:1 | 1 (-1.61325) | -1 | -1 |
| G: -5312.08193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11578.02202 HOMO: -6.77019 LUMO: -1.03131 factor:1 | 1 (-1.57440) | -1 | -1 |
| G: -5312.08193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11578.21381 HOMO: -6.80285 LUMO: 1.05852 factor:1 | 1 (-1.76618) | -1 | -1 |
| G: -5312.08193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.77380 HOMO: -6.76475 LUMO: 1.01771 factor:1 | 1 (-1.32617) | -1 | -1 |
| G: -5312.08193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11578.00850 HOMO: -6.92530 LUMO: 1.37417 factor:1 | 1 (-1.56087) | -1 | -1 |
| G: -5312.08193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.95089 HOMO: -6.98244 LUMO: 1.25989 factor:1 | 1 (-1.50327) | -1 | -1 |
| G: -5312.08193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11578.06075 HOMO: -6.74842 LUMO: 0.89798 factor:1 | 1 (-1.61312) | -1 | -1 |
| G: -5312.08193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.89399 HOMO: -6.77019 LUMO: -1.17009 factor:1 | 1 (-1.44637) | -1 | -1 |
| G: -5312.08193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11578.14146 HOMO: -6.78652 LUMO: 1.35785 factor:1 | 1 (-1.69383) | -1 | -1 |
| G: -5312.08193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.70452 HOMO: -6.82734 LUMO: -0.68301 factor:1 | 1 (-1.25689) | -1 | -1 |
| G: -5312.08193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.86997 HOMO: -6.48175 LUMO: -2.19052 factor:1 | 1 (-1.42234) | -1 | -1 |
| G: -5312.08193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.77571 HOMO: -6.65863 LUMO: -0.77008 factor:1 | 1 (-1.32808) | -1 | -1 |
| G: -5312.08193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.81361 HOMO: -6.44094 LUMO: -2.20956 factor:1 | 1 (-1.36598) | -1 | -1 |
| G: -5312.08193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.86338 HOMO: -6.59876 LUMO: -0.57688 factor:1 | 1 (-1.41575) | -1 | -1 |
| G: -5312.08193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11578.22701 HOMO: -6.78380 LUMO: -0.77008 factor:1 | 1 (-1.77938) | -1 | -1 |
| G: -5312.08193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11578.04143 HOMO: -7.30354 LUMO: 0.25034 factor:1 | 1 (-1.59380) | -1 | -1 |
| G: -5312.08193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11578.00494 HOMO: -6.59332 LUMO: -0.53334 factor:1 | 1 (-1.55731) | -1 | -1 |
| G: -5312.08193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.23273 HOMO: -6.64230 LUMO: -0.55783 factor:1 | 1 (-0.78510) | -1 | -1 |
| G: -5312.08193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.31940 HOMO: -7.26544 LUMO: 0.20409 factor:1 | 1 (-0.87177) | -1 | -1 |
| G: -5312.08193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.90151 HOMO: -6.61237 LUMO: -0.65307 factor:1 | 1 (-0.45389) | -1 | -1 |
| G: -5312.08193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.00786 HOMO: -6.72393 LUMO: -0.65307 factor:1 | 1 (-0.56023) | -1 | -1 |
| G: -5312.08193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.24511 HOMO: -6.29671 LUMO: -0.39729 factor:1 | 1 (-0.79748) | -1 | -1 |
| G: -5312.08193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.43682 HOMO: -6.75387 LUMO: -0.53334 factor:1 | 1 (-0.98919) | -1 | -1 |
| G: -5312.08193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.83966 HOMO: -6.53073 LUMO: -0.31293 factor:1 | 1 (-0.39203) | -1 | -1 |
| G: -5312.08193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.07820 HOMO: -6.42189 LUMO: -0.59049 factor:1 | 1 (-0.63057) | -1 | -1 |
| G: -5312.08193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.27589 HOMO: -6.41100 LUMO: -0.29933 factor:1 | 1 (-0.82826) | -1 | -1 |
| G: -5312.08193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.84099 HOMO: -6.57427 LUMO: -0.53879 factor:1 | 1 (-1.39336) | -1 | -1 |
| G: -5312.08193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.84602 HOMO: -7.43143 LUMO: 0.33470 factor:1 | 1 (-1.39839) | -1 | -1 |
| G: -5312.08193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.77715 HOMO: -6.56067 LUMO: -0.50885 factor:1 | 1 (-1.32952) | -1 | -1 |
| G: -5312.08193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.77601 HOMO: -6.65863 LUMO: -0.76464 factor:1 | 1 (-1.32838) | -1 | -1 |
| G: -5312.08193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.84099 HOMO: -6.32665 LUMO: -0.41906 factor:1 | 1 (-1.39336) | -1 | -1 |
| G: -5312.08193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.76071 HOMO: -6.57699 LUMO: 1.63813 factor:1 | 1 (-1.31309) | -1 | -1 |
| G: -5312.08193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.82929 HOMO: -6.53073 LUMO: 1.71704 factor:1 | 1 (-1.38166) | -1 | -1 |
| G: -5312.08193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.83998 HOMO: -6.86271 LUMO: 2.07351 factor:1 | 1 (-1.39235) | -1 | -1 |
| G: -5312.08193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11578.06382 HOMO: -6.63686 LUMO: 1.78235 factor:1 | 1 (-1.61619) | -1 | -1 |
| G: -5312.08193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11578.05656 HOMO: -6.60965 LUMO: 1.94289 factor:1 | 1 (-1.60893) | -1 | -1 |
| G: -5312.08193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.78877 HOMO: -6.55250 LUMO: 1.89119 factor:1 | 1 (-1.34114) | -1 | -1 |
| G: -5312.08193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.94172 HOMO: -6.50624 LUMO: 1.85582 factor:1 | 1 (-1.49410) | -1 | -1 |
| G: -5312.08193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.96847 HOMO: -6.06814 LUMO: 1.94561 factor:1 | 1 (-1.52084) | -1 | -1 |
| G: -5312.08193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.95070 HOMO: -6.58788 LUMO: 2.01908 factor:1 | 1 (-1.50308) | -1 | -1 |
| G: -5312.08193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.86142 HOMO: -6.74026 LUMO: 0.31293 factor:1 | 1 (-1.41379) | -1 | -1 |
| G: -5312.08193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.97636 HOMO: -6.54434 LUMO: -0.42994 factor:1 | 1 (-1.52874) | -1 | -1 |
| G: -5312.08193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.71573 HOMO: -6.94707 LUMO: 0.42994 factor:1 | 1 (-1.26811) | -1 | -1 |
| G: -5312.08193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11578.05544 HOMO: -6.98516 LUMO: 0.41361 factor:1 | 1 (-1.60781) | -1 | -1 |
| G: -5312.08193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11578.06317 HOMO: -6.31304 LUMO: -0.54967 factor:1 | 1 (-1.61554) | -1 | -1 |
| G: -5312.08193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11578.09218 HOMO: -6.48447 LUMO: -0.40817 factor:1 | 1 (-1.64455) | -1 | -1 |
| G: -5312.08193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.77130 HOMO: -6.49264 LUMO: 0.29116 factor:1 | 1 (-1.32367) | -1 | -1 |
| G: -5312.08193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.76115 HOMO: -6.48719 LUMO: -0.11973 factor:1 | 1 (-1.31352) | -1 | -1 |
| G: -5312.08193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11578.03054 HOMO: -7.16204 LUMO: 0.44082 factor:1 | 1 (-1.58291) | -1 | -1 |
| G: -5312.08193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.76855 HOMO: -6.74842 LUMO: -0.37552 factor:1 | 1 (-1.32092) | -1 | -1 |
| G: -5312.08193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.89979 HOMO: -6.44638 LUMO: -0.45171 factor:1 | 1 (-1.45216) | -1 | -1 |
| G: -5312.08193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.75244 HOMO: -7.07496 LUMO: 0.50341 factor:1 | 1 (-1.30481) | -1 | -1 |
| G: -5312.08193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.68357 HOMO: -6.79468 LUMO: 0.11429 factor:1 | 1 (-1.23594) | -1 | -1 |
| G: -5312.08193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.96059 HOMO: -6.63958 LUMO: -0.67484 factor:1 | 1 (-0.51296) | -1 | -1 |
| G: -5312.08193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.28223 HOMO: -7.08584 LUMO: 0.46259 factor:1 | 1 (-0.83460) | -1 | -1 |
| G: -5312.08193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.07545 HOMO: -6.80285 LUMO: -0.73199 factor:1 | 1 (-0.62782) | -1 | -1 |
| G: -5312.08193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.03052 HOMO: -6.44366 LUMO: -0.45443 factor:1 | 1 (-0.58290) | -1 | -1 |
| G: -5312.08193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.86180 HOMO: -6.75931 LUMO: 0.25851 factor:1 | 1 (-1.41418) | -1 | -1 |
| G: -5312.08193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.72137 HOMO: -6.64502 LUMO: 1.79323 factor:1 | 1 (-1.27374) | -1 | -1 |
| G: -5312.08193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11578.10442 HOMO: -6.51168 LUMO: 1.60275 factor:1 | 1 (-1.65679) | -1 | -1 |
| G: -5312.08193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.94834 HOMO: -6.56067 LUMO: 1.63268 factor:1 | 1 (-1.50071) | -1 | -1 |
| G: -5312.08193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.93908 HOMO: -6.56883 LUMO: 1.70615 factor:1 | 1 (-1.49146) | -1 | -1 |
| G: -5312.08193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11578.05239 HOMO: -6.77836 LUMO: 1.77962 factor:1 | 1 (-1.60476) | -1 | -1 |
| G: -5312.08193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.78537 HOMO: -6.38923 LUMO: 1.85854 factor:1 | 1 (-1.33774) | -1 | -1 |
| G: -5312.08193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.85157 HOMO: -6.35658 LUMO: 2.16875 factor:1 | 1 (-1.40394) | -1 | -1 |
| G: -5312.08193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11578.03854 HOMO: -6.83006 LUMO: 2.31025 factor:1 | 1 (-1.59091) | -1 | -1 |
| G: -5312.08193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11578.06763 HOMO: -6.87087 LUMO: 1.79051 factor:1 | 1 (-1.62000) | -1 | -1 |
| G: -5312.08193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11578.09294 HOMO: -6.56339 LUMO: 2.37828 factor:1 | 1 (-1.64531) | -1 | -1 |
| G: -5312.08193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.93631 HOMO: -6.30488 LUMO: 2.51705 factor:1 | 1 (-1.48868) | -1 | -1 |
| G: -5312.08193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.77212 HOMO: -6.69400 LUMO: 1.95650 factor:1 | 1 (-1.32449) | -1 | -1 |
| G: -5312.08193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.61630 HOMO: -6.51168 LUMO: 2.03541 factor:1 | 1 (-1.16867) | -1 | -1 |
| G: -5312.08193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.80455 HOMO: -6.30760 LUMO: 1.65173 factor:1 | 1 (-1.35692) | -1 | -1 |
| G: -5312.08193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.87865 HOMO: -6.55250 LUMO: 1.90752 factor:1 | 1 (-1.43102) | -1 | -1 |
| G: -5312.08193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.74014 HOMO: -6.41372 LUMO: 1.76058 factor:1 | 1 (-1.29251) | -1 | -1 |
| G: -5312.08193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.56972 HOMO: -6.23957 LUMO: 2.06534 factor:1 | 1 (-1.12209) | -1 | -1 |
| G: -5312.08193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.44552 HOMO: -6.58243 LUMO: 2.11705 factor:1 | 1 (-0.99790) | -1 | -1 |
| G: -5312.08193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.59935 HOMO: -6.37835 LUMO: 2.09256 factor:1 | 1 (-1.15172) | -1 | -1 |
| G: -5312.08193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.52329 HOMO: -6.50624 LUMO: 2.55787 factor:1 | 1 (-1.07567) | -1 | -1 |
| G: -5312.08193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.71383 HOMO: -6.45454 LUMO: 1.87214 factor:1 | 1 (-1.26620) | -1 | -1 |
| G: -5312.08193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.42596 HOMO: -6.53617 LUMO: 1.95650 factor:1 | 1 (-0.97833) | -1 | -1 |
| G: -5312.08193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.65685 HOMO: -6.51985 LUMO: 1.71432 factor:1 | 1 (-1.20922) | -1 | -1 |
| G: -5312.08193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.50610 HOMO: -6.75114 LUMO: 1.84493 factor:1 | 1 (-1.05847) | -1 | -1 |
| G: -5312.08193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.60893 HOMO: -6.06270 LUMO: 1.65717 factor:1 | 1 (-1.16130) | -1 | -1 |
| G: -5312.08193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.82452 HOMO: -5.89671 LUMO: 1.71704 factor:1 | 1 (-1.37690) | -1 | -1 |
| G: -5312.08193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.53584 HOMO: -6.18787 LUMO: 1.91840 factor:1 | 1 (-1.08821) | -1 | -1 |
| G: -5312.08193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.48803 HOMO: -6.01644 LUMO: 1.85582 factor:1 | 1 (-1.04040) | -1 | -1 |
| G: -5312.08193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.43894 HOMO: -6.05998 LUMO: 2.33474 factor:1 | 1 (-0.99131) | -1 | -1 |
| G: -5312.08193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.72343 HOMO: -6.05725 LUMO: 2.03541 factor:1 | 1 (-1.27581) | -1 | -1 |
| G: -5312.08193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.63081 HOMO: -6.80829 LUMO: 1.90480 factor:1 | 1 (-1.18318) | -1 | -1 |
| G: -5312.08193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.70928 HOMO: -6.76475 LUMO: 2.20956 factor:1 | 1 (-1.26166) | -1 | -1 |
| G: -5312.08193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.74349 HOMO: -6.29944 LUMO: 1.77962 factor:1 | 1 (-1.29586) | -1 | -1 |
| G: -5312.08193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.83481 HOMO: -6.47359 LUMO: -0.25579 factor:1 | 1 (-1.38718) | -1 | -1 |
| G: -5312.08193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11578.05411 HOMO: -6.57699 LUMO: -0.47348 factor:1 | 1 (-1.60648) | -1 | -1 |
| G: -5312.08193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.79761 HOMO: -7.20830 LUMO: 0.49797 factor:1 | 1 (-1.34998) | -1 | -1 |
| G: -5312.08193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.76428 HOMO: -7.49402 LUMO: 0.29933 factor:1 | 1 (-1.31665) | -1 | -1 |
| G: -5312.08193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.75108 HOMO: -6.66679 LUMO: -0.58777 factor:1 | 1 (-1.30345) | -1 | -1 |
| G: -5312.08193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.91136 HOMO: -6.67767 LUMO: -0.56328 factor:1 | 1 (-1.46373) | -1 | -1 |
| G: -5312.08193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.70488 HOMO: -7.42871 LUMO: 0.35647 factor:1 | 1 (-1.25725) | -1 | -1 |
| G: -5312.08193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.78934 HOMO: -6.56067 LUMO: -0.54423 factor:1 | 1 (-1.34171) | -1 | -1 |
| G: -5312.08193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.48343 HOMO: -6.56339 LUMO: -0.50341 factor:1 | 1 (-1.03580) | -1 | -1 |
| G: -5312.08193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.43818 HOMO: -6.56067 LUMO: -0.48436 factor:1 | 1 (-0.99055) | -1 | -1 |
| G: -5312.08193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.54229 HOMO: -6.73210 LUMO: 1.75241 factor:1 | 1 (-1.09466) | -1 | -1 |
| G: -5312.08193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.43543 HOMO: -6.48175 LUMO: 1.91296 factor:1 | 1 (-0.98780) | -1 | -1 |
| G: -5312.08193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.34990 HOMO: -6.67767 LUMO: 1.70343 factor:1 | 1 (-0.90228) | -1 | -1 |
| G: -5312.08193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.39061 HOMO: -6.37835 LUMO: 1.96466 factor:1 | 1 (-0.94298) | -1 | -1 |
| G: -5312.08193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.64136 HOMO: -6.40828 LUMO: 2.10072 factor:1 | 1 (-1.19374) | -1 | -1 |
| G: -5312.08193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.42732 HOMO: -6.06542 LUMO: 1.92112 factor:1 | 1 (-0.97969) | -1 | -1 |
| G: -5312.08193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.73405 HOMO: -6.90353 LUMO: 1.83133 factor:1 | 1 (-1.28642) | -1 | -1 |
| G: -5312.08193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.48950 HOMO: -6.37019 LUMO: 1.92929 factor:1 | 1 (-1.04187) | -1 | -1 |
| G: -5312.08193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.33015 HOMO: -6.61509 LUMO: 2.11160 factor:1 | 1 (-0.88252) | -1 | -1 |
| G: -5312.08193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.27763 HOMO: -6.82734 LUMO: 1.77146 factor:1 | 1 (-0.83000) | -1 | -1 |
| G: -5312.08193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.17774 HOMO: -6.01100 LUMO: 1.89935 factor:1 | 1 (-0.73011) | -1 | -1 |
| G: -5312.08193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.93550 HOMO: -6.49536 LUMO: 1.75241 factor:1 | 1 (-0.48787) | -1 | -1 |
| G: -5312.08193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.42231 HOMO: -6.34297 LUMO: 1.86398 factor:1 | 1 (-0.97468) | -1 | -1 |
| G: -5312.08193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.22381 HOMO: -6.53073 LUMO: 1.84493 factor:1 | 1 (-0.77618) | -1 | -1 |
| G: -5312.08193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.11708 HOMO: -6.53345 LUMO: 2.41093 factor:1 | 1 (-0.66945) | -1 | -1 |
| G: -5312.08193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.60969 HOMO: -7.01237 LUMO: 2.06262 factor:1 | 1 (-1.16206) | -1 | -1 |
| G: -5312.08193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.16239 HOMO: -6.17154 LUMO: 1.89119 factor:1 | 1 (-0.71476) | -1 | -1 |
| G: -5312.08193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.27962 HOMO: -6.08719 LUMO: 1.74425 factor:1 | 1 (-0.83199) | -1 | -1 |
| G: -5312.08193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.36359 HOMO: -6.69672 LUMO: 1.95106 factor:1 | 1 (-0.91596) | -1 | -1 |
| G: -5312.08193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11578.11743 HOMO: -6.58243 LUMO: 2.24766 factor:1 | 1 (-1.66980) | -1 | -1 |
| G: -5312.08193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11578.01816 HOMO: -6.74570 LUMO: 2.02181 factor:1 | 1 (-1.57053) | -1 | -1 |
| G: -5312.08193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11578.34641 HOMO: -6.53890 LUMO: 1.92929 factor:1 | 1 (-1.89878) | -1 | -1 |
| G: -5312.08193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.81614 HOMO: -6.03276 LUMO: 1.67078 factor:1 | 1 (-1.36852) | -1 | -1 |
| G: -5312.08193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11578.72579 HOMO: -6.67767 LUMO: 2.03541 factor:1 | 1 (-2.27816) | -1 | -1 |
| G: -5312.08193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11578.20976 HOMO: -5.98378 LUMO: 1.84221 factor:1 | 1 (-1.76213) | -1 | -1 |
| G: -5312.08193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11578.40336 HOMO: -6.07086 LUMO: 2.01908 factor:1 | 1 (-1.95574) | -1 | -1 |
| G: -5312.08193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11578.39887 HOMO: -6.29944 LUMO: 1.90208 factor:1 | 1 (-1.95125) | -1 | -1 |
| G: -5312.08193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11578.77831 HOMO: -6.75114 LUMO: 1.85854 factor:1 | 1 (-2.33068) | -1 | -1 |
| G: -5312.08193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11578.21773 HOMO: -6.56611 LUMO: 2.49801 factor:1 | 1 (-1.77010) | -1 | -1 |
| G: -5312.08193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11578.53074 HOMO: -6.39740 LUMO: 1.92929 factor:1 | 1 (-2.08311) | -1 | -1 |
| G: -5312.08193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11579.08836 HOMO: -6.85999 LUMO: -1.07757 factor:1 | 1 (-2.64073) | -1 | -1 |
| G: -5312.08193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11578.82120 HOMO: -6.98244 LUMO: 1.07213 factor:1 | 1 (-2.37357) | -1 | -1 |
| G: -5312.08193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11578.27542 HOMO: -7.04231 LUMO: 0.64219 factor:1 | 1 (-1.82779) | -1 | -1 |
| G: -5312.08193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11578.38184 HOMO: -6.96339 LUMO: 0.75648 factor:1 | 1 (-1.93421) | -1 | -1 |
| G: -5312.08193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11578.16682 HOMO: -6.83822 LUMO: -0.97417 factor:1 | 1 (-1.71919) | -1 | -1 |
| G: -5312.08193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11579.02120 HOMO: -6.44910 LUMO: -2.15242 factor:1 | 1 (-2.57357) | -1 | -1 |
| G: -5312.08193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11578.83913 HOMO: -6.84094 LUMO: -1.37690 factor:1 | 1 (-2.39150) | -1 | -1 |
| G: -5312.08193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11578.03351 HOMO: -6.74026 LUMO: -2.54699 factor:1 | 1 (-1.58588) | -1 | -1 |
| G: -5312.08193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11578.23299 HOMO: -6.96611 LUMO: 1.24900 factor:1 | 1 (-1.78537) | -1 | -1 |
| G: -5312.08193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.84477 HOMO: -7.21102 LUMO: 0.82995 factor:1 | 1 (-1.39714) | -1 | -1 |
| G: -5312.08193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.79947 HOMO: -6.88448 LUMO: 0.81634 factor:1 | 1 (-0.35184) | -1 | -1 |
| G: -5312.08193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.84769 HOMO: -7.04231 LUMO: 1.10750 factor:1 | 1 (-0.40006) | -1 | -1 |
| G: -5312.08193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.86249 HOMO: -6.83550 LUMO: -0.98777 factor:1 | 1 (-0.41486) | -1 | -1 |
| G: -5312.08193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.62652 HOMO: -6.82189 LUMO: 0.93879 factor:1 | 1 (-0.17889) | -1 | -1 |
| G: -5312.08193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.73604 HOMO: -6.81101 LUMO: 0.70750 factor:1 | 1 (-0.28841) | -1 | -1 |
| G: -5312.08193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.66398 HOMO: -7.06680 LUMO: 0.74015 factor:1 | 1 (-1.21635) | -1 | -1 |
| G: -5312.08193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.89965 HOMO: -6.68856 LUMO: 0.86260 factor:1 | 1 (-1.45203) | -1 | -1 |
| G: -5312.08193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.91835 HOMO: -6.83822 LUMO: -0.63403 factor:1 | 1 (-1.47072) | -1 | -1 |
| G: -5312.08193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.59715 HOMO: -6.84911 LUMO: 1.26533 factor:1 | 1 (-1.14952) | -1 | -1 |
| G: -5312.08193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.86385 HOMO: -7.01237 LUMO: 0.73743 factor:1 | 1 (-0.41623) | -1 | -1 |
| G: -5312.08193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.86021 HOMO: -7.00965 LUMO: 1.40139 factor:1 | 1 (-0.41258) | -1 | -1 |
| G: -5312.08193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.02035 HOMO: -6.73210 LUMO: -2.49256 factor:1 | 1 (-0.57272) | -1 | -1 |
| G: -5312.08193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.22378 HOMO: -7.08040 LUMO: 0.84627 factor:1 | 1 (-0.77615) | -1 | -1 |
| G: -5312.08193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.09305 HOMO: -7.00965 LUMO: 0.82995 factor:1 | 1 (-0.64543) | -1 | -1 |
| G: -5312.08193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.71770 HOMO: -6.88448 LUMO: 0.82723 factor:1 | 1 (-0.27007) | -1 | -1 |
| G: -5312.08193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.80674 HOMO: -7.20013 LUMO: 0.88437 factor:1 | 1 (-0.35911) | -1 | -1 |
| G: -5312.08193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.72845 HOMO: -6.60420 LUMO: -0.53334 factor:1 | 1 (-0.28082) | -1 | -1 |
| G: -5312.08193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.05586 HOMO: -6.78652 LUMO: -0.79729 factor:1 | 1 (-0.60823) | -1 | -1 |
| G: -5312.08193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.82402 HOMO: -6.48992 LUMO: -0.64491 factor:1 | 1 (-0.37639) | -1 | -1 |
| G: -5312.08193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.98347 HOMO: -6.85999 LUMO: -0.78097 factor:1 | 1 (-0.53585) | -1 | -1 |
| G: -5312.08193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.21616 HOMO: -6.65046 LUMO: -0.78097 factor:1 | 1 (-0.76853) | -1 | -1 |
| G: -5312.08193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.55585 HOMO: -7.24095 LUMO: 0.37280 factor:1 | 1 (-0.10822) | -1 | -1 |
| G: -5312.08193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.69454 HOMO: -6.81101 LUMO: -0.74831 factor:1 | 1 (-0.24692) | -1 | -1 |
| G: -5312.08193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.89047 HOMO: -6.69400 LUMO: -0.77280 factor:1 | 1 (-0.44284) | -1 | -1 |
| G: -5312.08193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.68799 HOMO: -6.08447 LUMO: -0.68573 factor:1 | 1 (-0.24036) | -1 | -1 |
| G: -5312.08193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.13257 HOMO: -6.66679 LUMO: -0.47076 factor:1 | 1 (-0.68494) | -1 | -1 |
| G: -5312.08193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.19061 HOMO: -6.97428 LUMO: -1.10750 factor:1 | 1 (-0.74298) | -1 | -1 |
| G: -5312.08193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.92418 HOMO: -6.69128 LUMO: -0.54151 factor:1 | 1 (-0.47655) | -1 | -1 |
| G: -5312.08193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.76323 HOMO: -6.53617 LUMO: -0.35375 factor:1 | 1 (-0.31560) | -1 | -1 |
| G: -5312.08193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.61057 HOMO: -6.75659 LUMO: -0.41361 factor:1 | 1 (-0.16294) | -1 | -1 |
| G: -5312.08193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11578.08398 HOMO: -6.69400 LUMO: -0.67484 factor:1 | 1 (-1.63636) | -1 | -1 |
| G: -5312.08193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11579.01891 HOMO: -6.89264 LUMO: -0.90886 factor:1 | 1 (-2.57129) | -1 | -1 |
| G: -5312.08193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11578.31131 HOMO: -6.56339 LUMO: -0.52518 factor:1 | 1 (-1.86368) | -1 | -1 |
| G: -5312.08193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11578.02292 HOMO: -6.45726 LUMO: -0.65852 factor:1 | 1 (-1.57529) | -1 | -1 |
| G: -5312.08193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.78320 HOMO: -6.80557 LUMO: -0.56600 factor:1 | 1 (-0.33557) | -1 | -1 |
| G: -5312.08193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.75087 HOMO: -7.19469 LUMO: -0.91702 factor:1 | 1 (-0.30324) | -1 | -1 |
| G: -5312.08193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.07145 HOMO: -6.41100 LUMO: 0.79185 factor:1 | 1 (-0.62382) | -1 | -1 |
| G: -5312.08193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.99123 HOMO: -6.39195 LUMO: 0.26123 factor:1 | 1 (-0.54360) | -1 | -1 |
| G: -5312.08193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.66284 HOMO: -6.78924 LUMO: 0.35919 factor:1 | 1 (-0.21521) | -1 | -1 |
| G: -5312.08193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.77301 HOMO: -6.50624 LUMO: 0.71838 factor:1 | 1 (-1.32538) | -1 | -1 |
| G: -5312.08193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11578.40494 HOMO: -6.68584 LUMO: -0.66124 factor:1 | 1 (-1.95731) | -1 | -1 |
| G: -5312.08193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.74382 HOMO: -6.45182 LUMO: -0.48980 factor:1 | 1 (-1.29619) | -1 | -1 |
| G: -5312.08193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.99171 HOMO: -7.18925 LUMO: -1.01498 factor:1 | 1 (-1.54408) | -1 | -1 |
| G: -5312.08193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.68654 HOMO: -7.18925 LUMO: -0.63130 factor:1 | 1 (-1.23891) | -1 | -1 |
| G: -5312.08193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.69530 HOMO: -6.66679 LUMO: -0.57960 factor:1 | 1 (-1.24767) | -1 | -1 |
| G: -5312.08193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.91348 HOMO: -6.44910 LUMO: -0.30205 factor:1 | 1 (-1.46585) | -1 | -1 |
| G: -5312.08193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.92741 HOMO: -7.23279 LUMO: 0.46804 factor:1 | 1 (-1.47978) | -1 | -1 |
| G: -5312.08193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.50670 HOMO: -6.92802 LUMO: -0.72927 factor:1 | 1 (-1.05907) | -1 | -1 |
| G: -5312.08193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11578.06241 HOMO: -6.83278 LUMO: -0.59321 factor:1 | 1 (-1.61478) | -1 | -1 |
| G: -5312.08193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.97402 HOMO: -7.44776 LUMO: 0.27211 factor:1 | 1 (-1.52640) | -1 | -1 |
| G: -5312.08193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11578.26331 HOMO: -6.80829 LUMO: -0.59865 factor:1 | 1 (-1.81568) | -1 | -1 |
| G: -5312.08193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.73931 HOMO: -6.63686 LUMO: -0.75103 factor:1 | 1 (-0.29168) | -1 | -1 |
| G: -5312.08193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.83144 HOMO: -6.73210 LUMO: -0.55511 factor:1 | 1 (-0.38382) | -1 | -1 |
| G: -5312.08193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.57781 HOMO: -6.50624 LUMO: 1.58642 factor:1 | 1 (-0.13018) | -1 | -1 |
| G: -5312.08193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.89564 HOMO: -6.79196 LUMO: 0.96328 factor:1 | 1 (-0.44801) | -1 | -1 |
| G: -5312.08193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.04369 HOMO: -6.82734 LUMO: 1.23540 factor:1 | 1 (-0.59607) | -1 | -1 |
| G: -5312.08193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.61098 HOMO: -6.90081 LUMO: 1.25444 factor:1 | 1 (-0.16335) | -1 | -1 |
| G: -5312.08193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11578.45460 HOMO: -7.00965 LUMO: -1.05036 factor:1 | 1 (-2.00698) | -1 | -1 |
| G: -5312.08193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.63078 HOMO: -7.01237 LUMO: -1.48302 factor:1 | 1 (-1.18315) | -1 | -1 |
| G: -5312.08193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.76730 HOMO: -6.91713 LUMO: 0.93607 factor:1 | 1 (-1.31967) | -1 | -1 |
| G: -5312.08193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.91810 HOMO: -7.02598 LUMO: 0.92247 factor:1 | 1 (-1.47048) | -1 | -1 |
| G: -5312.08193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11578.14880 HOMO: -6.98516 LUMO: 1.52384 factor:1 | 1 (-1.70117) | -1 | -1 |
| G: -5312.08193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11578.33079 HOMO: -6.75387 LUMO: 1.04764 factor:1 | 1 (-1.88316) | -1 | -1 |
| G: -5312.08193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11578.37721 HOMO: -7.09401 LUMO: 1.19458 factor:1 | 1 (-1.92959) | -1 | -1 |
| G: -5312.08193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.91239 HOMO: -6.88992 LUMO: -1.56193 factor:1 | 1 (-1.46476) | -1 | -1 |
| G: -5312.08193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.64634 HOMO: -7.00149 LUMO: 0.99866 factor:1 | 1 (-1.19872) | -1 | -1 |
| G: -5312.08193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.88866 HOMO: -7.13755 LUMO: 1.05308 factor:1 | 1 (-1.44103) | -1 | -1 |
| G: -5312.08193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.93949 HOMO: -6.85183 LUMO: -1.42860 factor:1 | 1 (-1.49186) | -1 | -1 |
| G: -5312.08193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.66830 HOMO: -6.63141 LUMO: -0.88981 factor:1 | 1 (-1.22068) | -1 | -1 |
| G: -5312.08193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11578.10924 HOMO: -6.92258 LUMO: -0.82178 factor:1 | 1 (-1.66161) | -1 | -1 |
| G: -5312.08193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11578.33316 HOMO: -6.55794 LUMO: -0.80818 factor:1 | 1 (-1.88553) | -1 | -1 |
| G: -5312.08193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11578.24845 HOMO: -6.95251 LUMO: -0.97145 factor:1 | 1 (-1.80082) | -1 | -1 |
| G: -5312.08193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11578.01057 HOMO: -7.37701 LUMO: 0.14150 factor:1 | 1 (-1.56294) | -1 | -1 |
| G: -5312.08193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.89724 HOMO: -6.74842 LUMO: -0.68028 factor:1 | 1 (-0.44961) | -1 | -1 |
| G: -5312.08193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.74214 HOMO: -6.65046 LUMO: -0.52518 factor:1 | 1 (-0.29451) | -1 | -1 |
| G: -5312.08193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.87251 HOMO: -6.91441 LUMO: -1.13199 factor:1 | 1 (-0.42488) | -1 | -1 |
| G: -5312.08193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.94647 HOMO: -7.00965 LUMO: -1.00682 factor:1 | 1 (-0.49884) | -1 | -1 |
| G: -5312.08193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.93477 HOMO: -6.55794 LUMO: -0.54967 factor:1 | 1 (-0.48714) | -1 | -1 |
| G: -5312.08193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.00935 HOMO: -6.71577 LUMO: -0.53879 factor:1 | 1 (-0.56172) | -1 | -1 |
| G: -5312.08193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.60404 HOMO: -6.88992 LUMO: -0.55511 factor:1 | 1 (-0.15641) | -1 | -1 |
| G: -5312.08193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.82151 HOMO: -6.74026 LUMO: -0.60681 factor:1 | 1 (-0.37388) | -1 | -1 |
| G: -5312.08193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.69709 HOMO: -6.76747 LUMO: -0.50885 factor:1 | 1 (-1.24947) | -1 | -1 |
| G: -5312.08193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11578.51531 HOMO: -6.87904 LUMO: -0.92519 factor:1 | 1 (-2.06768) | -1 | -1 |
| G: -5312.08193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.89508 HOMO: -6.53073 LUMO: -0.53062 factor:1 | 1 (-1.44746) | -1 | -1 |
| G: -5312.08193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.93759 HOMO: -6.97700 LUMO: -0.98505 factor:1 | 1 (-1.48996) | -1 | -1 |
| G: -5312.08193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.63894 HOMO: -6.96884 LUMO: -0.79185 factor:1 | 1 (-1.19131) | -1 | -1 |
| G: -5312.08193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.71595 HOMO: -6.60420 LUMO: -0.31021 factor:1 | 1 (-1.26832) | -1 | -1 |
| G: -5312.08193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.60123 HOMO: -6.68584 LUMO: -0.63947 factor:1 | 1 (-1.15360) | -1 | -1 |
| G: -5312.08193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.75565 HOMO: -6.41917 LUMO: -0.35103 factor:1 | 1 (-1.30802) | -1 | -1 |
| G: -5312.08193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.65124 HOMO: -6.73482 LUMO: -0.70477 factor:1 | 1 (-1.20361) | -1 | -1 |
| G: -5312.08193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.98387 HOMO: -6.71305 LUMO: -0.85716 factor:1 | 1 (-1.53625) | -1 | -1 |
| G: -5312.08193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.89887 HOMO: -6.70761 LUMO: -0.63403 factor:1 | 1 (-0.45125) | -1 | -1 |
| G: -5312.08193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.09417 HOMO: -6.37563 LUMO: -0.38640 factor:1 | 1 (-0.64654) | -1 | -1 |
| G: -5312.08193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.98334 HOMO: -6.27495 LUMO: -0.54967 factor:1 | 1 (-0.53571) | -1 | -1 |
| G: -5312.08193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.03205 HOMO: -6.98516 LUMO: 0.38096 factor:1 | 1 (-0.58442) | -1 | -1 |
| G: -5312.08193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.01289 HOMO: -6.47087 LUMO: -0.40001 factor:1 | 1 (-0.56526) | -1 | -1 |
| G: -5312.08193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.98630 HOMO: -6.59876 LUMO: 0.20681 factor:1 | 1 (-0.53868) | -1 | -1 |
| G: -5312.08193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.23306 HOMO: -6.89809 LUMO: 0.14966 factor:1 | 1 (-0.78543) | -1 | -1 |
| G: -5312.08193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.17899 HOMO: -6.76203 LUMO: 2.11432 factor:1 | 1 (-0.73136) | -1 | -1 |
| G: -5312.08193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.77172 HOMO: -6.58516 LUMO: 1.75786 factor:1 | 1 (-0.32409) | -1 | -1 |
| G: -5312.08193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.86576 HOMO: -6.37835 LUMO: 1.84493 factor:1 | 1 (-0.41813) | -1 | -1 |
| G: -5312.08193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.77947 HOMO: -6.83550 LUMO: 1.74425 factor:1 | 1 (-0.33184) | -1 | -1 |
| G: -5312.08193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.99703 HOMO: -6.65318 LUMO: 1.79051 factor:1 | 1 (-0.54940) | -1 | -1 |
| G: -5312.08193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.72744 HOMO: -6.68584 LUMO: 2.11160 factor:1 | 1 (-0.27981) | -1 | -1 |
| G: -5312.08193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.03088 HOMO: -6.36202 LUMO: 1.85037 factor:1 | 1 (-0.58325) | -1 | -1 |
| G: -5312.08193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.98870 HOMO: -6.68312 LUMO: 2.23133 factor:1 | 1 (-0.54107) | -1 | -1 |
| G: -5312.08193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.95659 HOMO: -6.66679 LUMO: 2.14154 factor:1 | 1 (-0.50896) | -1 | -1 |
| G: -5312.08193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.06827 HOMO: -6.50896 LUMO: 1.92657 factor:1 | 1 (-0.62064) | -1 | -1 |
| G: -5312.08193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.91120 HOMO: -6.63686 LUMO: 2.22317 factor:1 | 1 (-0.46357) | -1 | -1 |
| G: -5312.08193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.25461 HOMO: -6.58788 LUMO: 2.17419 factor:1 | 1 (-0.80698) | -1 | -1 |
| G: -5312.08193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.89262 HOMO: -6.72665 LUMO: 2.12249 factor:1 | 1 (-0.44499) | -1 | -1 |
| G: -5312.08193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.63503 HOMO: -6.28311 LUMO: 1.91024 factor:1 | 1 (-0.18740) | -1 | -1 |
| G: -5312.08193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.90687 HOMO: -6.56067 LUMO: 2.27487 factor:1 | 1 (-0.45925) | -1 | -1 |
| G: -5312.08193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.69424 HOMO: -6.83006 LUMO: 2.28031 factor:1 | 1 (-0.24662) | -1 | -1 |
| G: -5312.08193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.97615 HOMO: -6.45182 LUMO: 1.62724 factor:1 | 1 (-0.52853) | -1 | -1 |
| G: -5312.08193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.05997 HOMO: -6.78380 LUMO: 1.83677 factor:1 | 1 (-0.61234) | -1 | -1 |
| G: -5312.08193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.75988 HOMO: -6.23413 LUMO: 1.80956 factor:1 | 1 (-0.31225) | -1 | -1 |
| G: -5312.08193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.98138 HOMO: -6.74298 LUMO: 2.16875 factor:1 | 1 (-0.53375) | -1 | -1 |
| G: -5312.08193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.89180 HOMO: -6.81645 LUMO: 2.50073 factor:1 | 1 (-0.44417) | -1 | -1 |
| G: -5312.08193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.85800 HOMO: -6.71033 LUMO: 1.96466 factor:1 | 1 (-0.41037) | -1 | -1 |
| G: -5312.08193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.76976 HOMO: -6.83550 LUMO: 2.04358 factor:1 | 1 (-0.32213) | -1 | -1 |
| G: -5312.08193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.49481 HOMO: -6.60965 LUMO: 2.38100 factor:1 | 1 (-0.04718) | -1 | -1 |
| G: -5312.08193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.62687 HOMO: -6.73210 LUMO: 2.26127 factor:1 | 1 (-0.17924) | -1 | -1 |
| G: -5312.08193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.54031 HOMO: -6.76203 LUMO: 2.13609 factor:1 | 1 (-0.09268) | -1 | -1 |
| G: -5312.08193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.89172 HOMO: -6.71033 LUMO: 2.05990 factor:1 | 1 (-0.44409) | -1 | -1 |
| G: -5312.08193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.98587 HOMO: -6.50896 LUMO: 2.32385 factor:1 | 1 (-0.53824) | -1 | -1 |
| G: -5312.08193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.88747 HOMO: -6.53345 LUMO: 1.74425 factor:1 | 1 (-0.43984) | -1 | -1 |
| G: -5312.08193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.07205 HOMO: -6.25862 LUMO: 1.63540 factor:1 | 1 (-0.62442) | -1 | -1 |
| G: -5312.08193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.73454 HOMO: -5.90759 LUMO: 1.78779 factor:1 | 1 (-0.28692) | -1 | -1 |
| G: -5312.08193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.13338 HOMO: -6.09807 LUMO: 1.99732 factor:1 | 1 (-0.68575) | -1 | -1 |
| G: -5312.08193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.00307 HOMO: -5.92392 LUMO: 1.99732 factor:1 | 1 (-0.55544) | -1 | -1 |
| G: -5312.08193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.07828 HOMO: -6.45182 LUMO: 1.72248 factor:1 | 1 (-0.63065) | -1 | -1 |
| G: -5312.08193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.34928 HOMO: -6.53073 LUMO: 1.82588 factor:1 | 1 (-0.90165) | -1 | -1 |
| G: -5312.08193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.16389 HOMO: -6.40828 LUMO: 2.05174 factor:1 | 1 (-0.71626) | -1 | -1 |
| G: -5312.08193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.98269 HOMO: -6.60420 LUMO: -0.82450 factor:1 | 1 (-0.53506) | -1 | -1 |
| G: -5312.08193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.92598 HOMO: -6.76747 LUMO: -0.57144 factor:1 | 1 (-0.47835) | -1 | -1 |
| G: -5312.08193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.99847 HOMO: -6.67767 LUMO: -0.59321 factor:1 | 1 (-0.55084) | -1 | -1 |
| G: -5312.08193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.17564 HOMO: -6.65863 LUMO: -0.57416 factor:1 | 1 (-0.72801) | -1 | -1 |
| G: -5312.08193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.10756 HOMO: -6.49808 LUMO: -0.54695 factor:1 | 1 (-0.65993) | -1 | -1 |
| G: -5312.08193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.14965 HOMO: -6.50080 LUMO: -0.61498 factor:1 | 1 (-0.70203) | -1 | -1 |
| G: -5312.08193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.28718 HOMO: -6.74842 LUMO: -0.51974 factor:1 | 1 (-0.83955) | -1 | -1 |
| G: -5312.08193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.83634 HOMO: -6.13345 LUMO: 0.67756 factor:1 | 1 (-0.38871) | -1 | -1 |
| G: -5312.08193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.87689 HOMO: -6.48719 LUMO: 0.52790 factor:1 | 1 (-0.42926) | -1 | -1 |
| G: -5312.08193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.76159 HOMO: -6.35930 LUMO: 0.74015 factor:1 | 1 (-0.31396) | -1 | -1 |
| G: -5312.08193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.96622 HOMO: -6.41644 LUMO: 0.22313 factor:1 | 1 (-0.51859) | -1 | -1 |
| G: -5312.08193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.91131 HOMO: -6.85727 LUMO: -0.00272 factor:1 | 1 (-0.46368) | -1 | -1 |
| G: -5312.08193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.75297 HOMO: -6.84638 LUMO: 0.24762 factor:1 | 1 (-0.30534) | -1 | -1 |
| G: -5312.08193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.09314 HOMO: -6.66951 LUMO: 0.39184 factor:1 | 1 (-0.64551) | -1 | -1 |
| G: -5312.08193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.01210 HOMO: -6.62597 LUMO: -0.65035 factor:1 | 1 (-0.56447) | -1 | -1 |
| G: -5312.08193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.00995 HOMO: -7.13755 LUMO: 0.45715 factor:1 | 1 (-0.56232) | -1 | -1 |
| G: -5312.08193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.68614 HOMO: -7.12666 LUMO: 0.45171 factor:1 | 1 (-0.23851) | -1 | -1 |
| G: -5312.08193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.64532 HOMO: -6.46270 LUMO: -0.46259 factor:1 | 1 (-0.19769) | -1 | -1 |
| G: -5312.08193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.46450 HOMO: -6.36202 LUMO: -0.29660 factor:1 | 1 (-0.01687) | -1 | -1 |
| G: -5312.08193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.57027 HOMO: -6.28583 LUMO: 0.40545 factor:1 | 1 (-0.12264) | -1 | -1 |
| G: -5312.08193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.93199 HOMO: -6.70761 LUMO: 0.41906 factor:1 | 1 (-0.48436) | -1 | -1 |
| G: -5312.08193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.86516 HOMO: -6.76203 LUMO: -0.60954 factor:1 | 1 (-0.41753) | -1 | -1 |
| G: -5312.08193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.87806 HOMO: -6.85999 LUMO: -0.75103 factor:1 | 1 (-0.43043) | -1 | -1 |
| G: -5312.08193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.01920 HOMO: -7.19741 LUMO: -1.00954 factor:1 | 1 (-0.57158) | -1 | -1 |
| G: -5312.08193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.99382 HOMO: -6.58243 LUMO: -0.33470 factor:1 | 1 (-0.54619) | -1 | -1 |
| G: -5312.08193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.21148 HOMO: -7.22190 LUMO: 0.49253 factor:1 | 1 (-0.76385) | -1 | -1 |
| G: -5312.08193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.05012 HOMO: -7.22462 LUMO: 0.51974 factor:1 | 1 (-0.60249) | -1 | -1 |
| G: -5312.08193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.05969 HOMO: -7.08584 LUMO: -0.68301 factor:1 | 1 (-0.61207) | -1 | -1 |
| G: -5312.08193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.91713 HOMO: -6.68584 LUMO: -0.29660 factor:1 | 1 (-0.46951) | -1 | -1 |
| G: -5312.08193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.74649 HOMO: -6.33753 LUMO: -0.48436 factor:1 | 1 (-0.29886) | -1 | -1 |
| G: -5312.08193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.71291 HOMO: -7.15932 LUMO: 0.55511 factor:1 | 1 (-0.26528) | -1 | -1 |
| G: -5312.08193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.62253 HOMO: -6.57427 LUMO: 2.01908 factor:1 | 1 (-1.17491) | -1 | -1 |
| G: -5312.08193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.46533 HOMO: -6.75659 LUMO: 2.22045 factor:1 | 1 (-1.01771) | -1 | -1 |
| G: -5312.08193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.58476 HOMO: -6.73482 LUMO: 2.20956 factor:1 | 1 (-1.13714) | -1 | -1 |
| G: -5312.08193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.75299 HOMO: -6.74026 LUMO: 1.76602 factor:1 | 1 (-1.30536) | -1 | -1 |
| G: -5312.08193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.85318 HOMO: -6.95523 LUMO: 1.94834 factor:1 | 1 (-1.40555) | -1 | -1 |
| G: -5312.08193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.64346 HOMO: -6.33209 LUMO: 1.87486 factor:1 | 1 (-1.19583) | -1 | -1 |
| G: -5312.08193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.48506 HOMO: -6.71033 LUMO: 2.12521 factor:1 | 1 (-1.03743) | -1 | -1 |
| G: -5312.08193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.33309 HOMO: -6.50080 LUMO: 2.04902 factor:1 | 1 (-0.88546) | -1 | -1 |
| G: -5312.08193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.73184 HOMO: -6.76475 LUMO: 1.94017 factor:1 | 1 (-1.28421) | -1 | -1 |
| G: -5312.08193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11578.19977 HOMO: -6.53073 LUMO: 2.08983 factor:1 | 1 (-1.75214) | -1 | -1 |
| G: -5312.08193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11578.08622 HOMO: -6.69944 LUMO: 2.20684 factor:1 | 1 (-1.63859) | -1 | -1 |
| G: -5312.08193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11578.23781 HOMO: -6.34570 LUMO: 1.80684 factor:1 | 1 (-1.79018) | -1 | -1 |
| G: -5312.08193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11578.80296 HOMO: -6.78380 LUMO: 1.95922 factor:1 | 1 (-2.35534) | -1 | -1 |
| G: -5312.08193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11579.10817 HOMO: -6.93618 LUMO: 1.76058 factor:1 | 1 (-2.66054) | -1 | -1 |
| G: -5312.08193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11578.32276 HOMO: -6.93346 LUMO: 1.79595 factor:1 | 1 (-1.87514) | -1 | -1 |
| G: -5312.08193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.77533 HOMO: -6.29671 LUMO: 1.75241 factor:1 | 1 (-1.32770) | -1 | -1 |
| G: -5312.08193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.98591 HOMO: -6.77019 LUMO: 1.74697 factor:1 | 1 (-1.53829) | -1 | -1 |
| G: -5312.08193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.87840 HOMO: -6.87360 LUMO: 1.91024 factor:1 | 1 (-1.43077) | -1 | -1 |
| G: -5312.08193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.97277 HOMO: -6.32665 LUMO: 1.87759 factor:1 | 1 (-1.52514) | -1 | -1 |
| G: -5312.08193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.69840 HOMO: -6.99877 LUMO: 1.99187 factor:1 | 1 (-1.25077) | -1 | -1 |
| G: -5312.08193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.94856 HOMO: -6.72665 LUMO: 2.12521 factor:1 | 1 (-0.50093) | -1 | -1 |
| G: -5312.08193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.87166 HOMO: -6.67767 LUMO: 2.43814 factor:1 | 1 (-0.42404) | -1 | -1 |
| G: -5312.08193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.90965 HOMO: -6.99605 LUMO: 1.79051 factor:1 | 1 (-0.46202) | -1 | -1 |
| G: -5312.08193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.00655 HOMO: -6.25046 LUMO: 1.77146 factor:1 | 1 (-0.55892) | -1 | -1 |
| G: -5312.08193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.11714 HOMO: -6.30488 LUMO: 1.90480 factor:1 | 1 (-0.66951) | -1 | -1 |
| G: -5312.08193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.12220 HOMO: -6.38379 LUMO: 1.68438 factor:1 | 1 (-0.67457) | -1 | -1 |
| G: -5312.08193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.85648 HOMO: -6.78924 LUMO: 2.01364 factor:1 | 1 (-0.40885) | -1 | -1 |
| G: -5312.08193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.81740 HOMO: -6.15249 LUMO: 1.98643 factor:1 | 1 (-0.36978) | -1 | -1 |
| G: -5312.08193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.81618 HOMO: -6.19331 LUMO: 2.14154 factor:1 | 1 (-0.36855) | -1 | -1 |
| G: -5312.08193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.95885 HOMO: -6.05998 LUMO: 2.12521 factor:1 | 1 (-0.51122) | -1 | -1 |
| G: -5312.08193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.83052 HOMO: -6.67223 LUMO: 1.91840 factor:1 | 1 (-0.38289) | -1 | -1 |
| G: -5312.08193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.01050 HOMO: -6.79196 LUMO: 2.18507 factor:1 | 1 (-0.56287) | -1 | -1 |
| G: -5312.08193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.80295 HOMO: -6.93346 LUMO: 1.78235 factor:1 | 1 (-0.35533) | -1 | -1 |
| G: -5312.08193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.01471 HOMO: -6.16882 LUMO: 1.80956 factor:1 | 1 (-0.56709) | -1 | -1 |
| G: -5312.08193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.19855 HOMO: -6.72665 LUMO: 2.07895 factor:1 | 1 (-0.75093) | -1 | -1 |
| G: -5312.08193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.72736 HOMO: -6.73210 LUMO: 1.97827 factor:1 | 1 (-0.27973) | -1 | -1 |
| G: -5312.08193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.88973 HOMO: -6.84638 LUMO: 1.87214 factor:1 | 1 (-0.44210) | -1 | -1 |
| G: -5312.08193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.88704 HOMO: -6.83006 LUMO: 2.36195 factor:1 | 1 (-0.43941) | -1 | -1 |
| G: -5312.08193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.73245 HOMO: -6.97700 LUMO: 1.91024 factor:1 | 1 (-0.28482) | -1 | -1 |
| G: -5312.08193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.97768 HOMO: -6.20420 LUMO: 1.81772 factor:1 | 1 (-0.53005) | -1 | -1 |
| G: -5312.08193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.81076 HOMO: -7.09129 LUMO: 2.10344 factor:1 | 1 (-0.36314) | 1 | 1 |
| G: -5312.08193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.05297 HOMO: -6.77564 LUMO: 2.14970 factor:1 | 1 (-0.60534) | -1 | -1 |
| G: -5312.08193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.90119 HOMO: -6.81645 LUMO: 1.85854 factor:1 | 1 (-0.45356) | -1 | -1 |
| G: -5312.08193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.74421 HOMO: -6.50896 LUMO: 2.04358 factor:1 | 1 (-0.29658) | -1 | -1 |
| G: -5312.08193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.64317 HOMO: -6.89264 LUMO: 1.66262 factor:1 | 1 (-0.19554) | -1 | -1 |
| G: -5312.08193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.00709 HOMO: -6.75931 LUMO: 2.23950 factor:1 | 1 (-0.55947) | -1 | -1 |
| G: -5312.08193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11578.18804 HOMO: -6.50080 LUMO: 1.67622 factor:1 | 1 (-1.74041) | -1 | -1 |
| G: -5312.08193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11578.94767 HOMO: -6.30216 LUMO: 2.24222 factor:1 | 1 (-2.50005) | -1 | -1 |
| G: -5312.08193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11578.05460 HOMO: -7.18108 LUMO: 2.10072 factor:1 | 1 (-1.60697) | 1 | 1 |
| G: -5312.08193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11578.37251 HOMO: -6.54162 LUMO: 2.35378 factor:1 | 1 (-1.92488) | -1 | -1 |
| G: -5312.08193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11578.11675 HOMO: -5.98650 LUMO: 1.48302 factor:1 | 1 (-1.66912) | -1 | -1 |
| G: -5312.08193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.80815 HOMO: -7.15115 LUMO: 2.14970 factor:1 | 1 (-0.36052) | 1 | 1 |
| G: -5312.08193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.66565 HOMO: -6.45454 LUMO: 2.15786 factor:1 | 1 (-0.21802) | -1 | -1 |
| G: -5312.08193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.82271 HOMO: -7.06952 LUMO: 2.14970 factor:1 | 1 (-0.37508) | 1 | 1 |
| G: -5312.08193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.76521 HOMO: -6.93618 LUMO: 1.86942 factor:1 | 1 (-0.31758) | -1 | -1 |
| G: -5312.08193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.98837 HOMO: -6.63141 LUMO: 1.92657 factor:1 | 1 (-0.54074) | -1 | -1 |
| G: -5312.08193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.71746 HOMO: -6.51441 LUMO: -0.44355 factor:1 | 1 (-0.26983) | -1 | -1 |
| G: -5312.08193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.72151 HOMO: -6.82734 LUMO: -1.03131 factor:1 | 1 (-0.27388) | -1 | -1 |
| G: -5312.08193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.47764 HOMO: -6.58788 LUMO: -0.82995 factor:1 | 1 (-0.03001) | -1 | -1 |
| G: -5312.08193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.97221 HOMO: -6.43277 LUMO: -0.40817 factor:1 | 1 (-0.52458) | -1 | -1 |
| G: -5312.08193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.79710 HOMO: -6.78924 LUMO: -0.72110 factor:1 | 1 (-1.34947) | -1 | -1 |
| G: -5312.08193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11578.39194 HOMO: -7.28177 LUMO: 0.36735 factor:1 | 1 (-1.94431) | -1 | -1 |
| G: -5312.08193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.66313 HOMO: -6.47903 LUMO: -0.46259 factor:1 | 1 (-1.21551) | -1 | -1 |
| G: -5312.08193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.80635 HOMO: -6.67495 LUMO: -0.75376 factor:1 | 1 (-1.35872) | -1 | -1 |
| G: -5312.08193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.96902 HOMO: -6.71033 LUMO: -0.71838 factor:1 | 1 (-1.52139) | -1 | -1 |
| G: -5312.08193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.70898 HOMO: -6.79740 LUMO: -0.79185 factor:1 | 1 (-1.26136) | -1 | -1 |
| G: -5312.08193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.65320 HOMO: -6.08719 LUMO: -0.63675 factor:1 | 1 (-1.20557) | -1 | -1 |
| G: -5312.08193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.97879 HOMO: -6.84094 LUMO: 0.42994 factor:1 | 1 (-1.53116) | -1 | -1 |
| G: -5312.08193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.60357 HOMO: -6.59604 LUMO: 0.25851 factor:1 | 1 (-1.15594) | -1 | -1 |
| G: -5312.08193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.78003 HOMO: -6.82462 LUMO: 0.08708 factor:1 | 1 (-1.33241) | -1 | -1 |
| G: -5312.08193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.99318 HOMO: -6.54706 LUMO: 0.44082 factor:1 | 1 (-1.54555) | -1 | -1 |
| G: -5312.08193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.89133 HOMO: -6.99333 LUMO: 0.32109 factor:1 | 1 (-1.44370) | -1 | -1 |
| G: -5312.08193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.64357 HOMO: -6.29944 LUMO: -0.57144 factor:1 | 1 (-1.19594) | -1 | -1 |
| G: -5312.08193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.71337 HOMO: -6.57699 LUMO: -0.46531 factor:1 | 1 (-1.26574) | -1 | -1 |
| G: -5312.08193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.56610 HOMO: -6.24773 LUMO: -0.53879 factor:1 | 1 (-1.11847) | -1 | -1 |
| G: -5312.08193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11578.20581 HOMO: -6.96067 LUMO: -0.67212 factor:1 | 1 (-1.75818) | -1 | -1 |
| G: -5312.08193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11578.78011 HOMO: -7.24095 LUMO: -0.09252 factor:1 | 1 (-2.33248) | -1 | -1 |
| G: -5312.08193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11578.16317 HOMO: -6.33481 LUMO: -0.46531 factor:1 | 1 (-1.71554) | -1 | -1 |
| G: -5312.08193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.93772 HOMO: -6.43549 LUMO: -0.33198 factor:1 | 1 (-1.49010) | -1 | -1 |
| G: -5312.08193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.96855 HOMO: -6.53073 LUMO: 0.44899 factor:1 | 1 (-1.52093) | -1 | -1 |
| G: -5312.08193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.74956 HOMO: -6.69128 LUMO: 0.47620 factor:1 | 1 (-1.30193) | -1 | -1 |
| G: -5312.08193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.61415 HOMO: -6.65318 LUMO: 0.52246 factor:1 | 1 (-1.16652) | -1 | -1 |
| G: -5312.08193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.65117 HOMO: -6.71305 LUMO: 0.41089 factor:1 | 1 (-0.20354) | -1 | -1 |
| G: -5312.08193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.87381 HOMO: -6.70216 LUMO: 0.19864 factor:1 | 1 (-0.42618) | -1 | -1 |
| G: -5312.08193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.86274 HOMO: -6.41100 LUMO: 0.34558 factor:1 | 1 (-0.41511) | -1 | -1 |
| G: -5312.08193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.77433 HOMO: -7.01237 LUMO: 0.02993 factor:1 | 1 (-0.32670) | -1 | -1 |
| G: -5312.08193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.75863 HOMO: -6.85999 LUMO: 0.18776 factor:1 | 1 (-0.31100) | -1 | -1 |
| G: -5312.08193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.69073 HOMO: -6.62869 LUMO: 0.48708 factor:1 | 1 (-0.24311) | -1 | -1 |
| G: -5312.08193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.88622 HOMO: -6.43821 LUMO: -0.45715 factor:1 | 1 (-0.43859) | -1 | -1 |
| G: -5312.08193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.68766 HOMO: -6.43277 LUMO: -0.72110 factor:1 | 1 (-0.24003) | -1 | -1 |
| G: -5312.08193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.96815 HOMO: -7.10761 LUMO: 0.43266 factor:1 | 1 (-0.52053) | -1 | -1 |
| G: -5312.08193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.72434 HOMO: -6.57699 LUMO: -0.61498 factor:1 | 1 (-0.27671) | -1 | -1 |
| G: -5312.08193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.81936 HOMO: -6.82189 LUMO: -0.75648 factor:1 | 1 (-0.37173) | -1 | -1 |
| G: -5312.08193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.56866 HOMO: -6.55794 LUMO: -0.67212 factor:1 | 1 (-0.12104) | -1 | -1 |
| G: -5312.08193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.96481 HOMO: -6.69128 LUMO: 1.88575 factor:1 | 1 (-0.51718) | -1 | -1 |
| G: -5312.08193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.69520 HOMO: -6.65591 LUMO: 1.70888 factor:1 | 1 (-0.24757) | -1 | -1 |
| G: -5312.08193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.60766 HOMO: -6.58788 LUMO: 1.68438 factor:1 | 1 (-0.16003) | -1 | -1 |
| G: -5312.08193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.55049 HOMO: -6.46270 LUMO: 1.72520 factor:1 | 1 (-0.10286) | -1 | -1 |
| G: -5312.08193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.70728 HOMO: -6.57427 LUMO: 1.73881 factor:1 | 1 (-0.25965) | -1 | -1 |
| G: -5312.08193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.79612 HOMO: -6.45182 LUMO: 1.75241 factor:1 | 1 (-0.34850) | -1 | -1 |
| G: -5312.08193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11578.01846 HOMO: -6.51441 LUMO: 1.78779 factor:1 | 1 (-1.57083) | -1 | -1 |
| G: -5312.08193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11579.11029 HOMO: -6.67495 LUMO: 2.11705 factor:1 | 1 (-2.66266) | -1 | -1 |
| G: -5312.08193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11578.18981 HOMO: -6.22597 LUMO: 1.96466 factor:1 | 1 (-1.74218) | -1 | -1 |
| G: -5312.08193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.64992 HOMO: -6.68040 LUMO: 2.30753 factor:1 | 1 (-0.20229) | -1 | -1 |
| G: -5312.08193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.78140 HOMO: -6.65046 LUMO: 2.18235 factor:1 | 1 (-0.33377) | -1 | -1 |
| G: -5312.08193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.79923 HOMO: -6.38651 LUMO: 1.76874 factor:1 | 1 (-0.35160) | -1 | -1 |
| G: -5312.08193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.64826 HOMO: -6.41644 LUMO: 2.09256 factor:1 | 1 (-0.20063) | -1 | -1 |
| G: -5312.08193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.81841 HOMO: -6.14977 LUMO: 2.28031 factor:1 | 1 (-0.37078) | -1 | -1 |
| G: -5312.08193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11578.35662 HOMO: -6.70489 LUMO: 2.43814 factor:1 | 1 (-1.90899) | -1 | -1 |
| G: -5312.08193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.73696 HOMO: -6.78924 LUMO: 2.27215 factor:1 | 1 (-1.28933) | -1 | -1 |
| G: -5312.08193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.65111 HOMO: -6.86271 LUMO: 2.31025 factor:1 | 1 (-1.20348) | -1 | -1 |
| G: -5312.08193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.76719 HOMO: -6.51168 LUMO: 2.04630 factor:1 | 1 (-1.31956) | -1 | -1 |
| G: -5312.08193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.73451 HOMO: -6.72665 LUMO: 2.13337 factor:1 | 1 (-1.28688) | -1 | -1 |
| G: -5312.08193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.85348 HOMO: -6.45998 LUMO: 2.16058 factor:1 | 1 (-1.40585) | -1 | -1 |
| G: -5312.08193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11578.54348 HOMO: -6.83822 LUMO: 2.20684 factor:1 | 1 (-2.09585) | -1 | -1 |
| G: -5312.08193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.61078 HOMO: -6.68856 LUMO: 2.19324 factor:1 | 1 (-1.16315) | -1 | -1 |
| G: -5312.08193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.94834 HOMO: -6.71577 LUMO: 2.16058 factor:1 | 1 (-0.50072) | -1 | -1 |
| G: -5312.08193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.11657 HOMO: -6.82462 LUMO: 1.90208 factor:1 | 1 (-0.66894) | -1 | -1 |
| G: -5312.08193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.05782 HOMO: -6.61509 LUMO: 2.23950 factor:1 | 1 (-0.61019) | -1 | -1 |
| G: -5312.08193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.05474 HOMO: -6.73754 LUMO: 1.84221 factor:1 | 1 (-0.60711) | -1 | -1 |
| G: -5312.08193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.01033 HOMO: -6.56611 LUMO: 1.94561 factor:1 | 1 (-0.56270) | -1 | -1 |
| G: -5312.08193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.11205 HOMO: -6.67767 LUMO: 1.51840 factor:1 | 1 (-0.66442) | -1 | -1 |
| G: -5312.08193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.89569 HOMO: -6.35658 LUMO: 2.16603 factor:1 | 1 (-0.44806) | -1 | -1 |
| G: -5312.08193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.76061 HOMO: -6.35114 LUMO: 2.08983 factor:1 | 1 (-0.31299) | -1 | -1 |
| G: -5312.08193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.28996 HOMO: -6.35114 LUMO: 2.10616 factor:1 | 1 (-0.84233) | -1 | -1 |
| G: -5312.08193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.12642 HOMO: -6.71305 LUMO: 2.01636 factor:1 | 1 (-0.67879) | -1 | -1 |
| G: -5312.08193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.16683 HOMO: -6.24773 LUMO: 1.98915 factor:1 | 1 (-0.71920) | -1 | -1 |
| G: -5312.08193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.12282 HOMO: -6.53617 LUMO: 2.42726 factor:1 | 1 (-0.67520) | -1 | -1 |
| G: -5312.08193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.26968 HOMO: -6.59332 LUMO: 1.82316 factor:1 | 1 (-0.82206) | -1 | -1 |
| G: -5312.08193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.27975 HOMO: -6.41372 LUMO: 1.77418 factor:1 | 1 (-0.83212) | -1 | -1 |
| G: -5312.08193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.99694 HOMO: -6.40284 LUMO: 1.88575 factor:1 | 1 (-0.54932) | -1 | -1 |
| G: -5312.08193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.02563 HOMO: -6.11168 LUMO: 1.70888 factor:1 | 1 (-0.57800) | -1 | -1 |
| G: -5312.08193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.49426 HOMO: -6.44910 LUMO: 2.23405 factor:1 | 1 (-1.04663) | -1 | -1 |
| G: -5312.08193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.27080 HOMO: -6.24773 LUMO: 2.12793 factor:1 | 1 (-0.82317) | -1 | -1 |
| G: -5312.08193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.21970 HOMO: -6.07358 LUMO: 1.89663 factor:1 | 1 (-0.77207) | -1 | -1 |
| G: -5312.08193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.41154 HOMO: -6.66679 LUMO: 1.96738 factor:1 | 1 (-0.96391) | -1 | -1 |
| G: -5312.08193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.12786 HOMO: -6.68312 LUMO: 1.78235 factor:1 | 1 (-0.68023) | -1 | -1 |
| G: -5312.08193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.03646 HOMO: -6.70761 LUMO: 1.97555 factor:1 | 1 (-0.58883) | -1 | -1 |
| G: -5312.08193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.04252 HOMO: -6.15794 LUMO: 2.00548 factor:1 | 1 (-0.59490) | -1 | -1 |
| G: -5312.08193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.17208 HOMO: -6.52257 LUMO: 1.96738 factor:1 | 1 (-0.72445) | -1 | -1 |
| G: -5312.08193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.27534 HOMO: -6.25590 LUMO: 1.86670 factor:1 | 1 (-0.82772) | -1 | -1 |
| G: -5312.08193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.19602 HOMO: -6.30216 LUMO: 1.84765 factor:1 | 1 (-0.74839) | -1 | -1 |
| G: -5312.08193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.34925 HOMO: -6.76747 LUMO: 2.20956 factor:1 | 1 (-0.90162) | -1 | -1 |
| G: -5312.08193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.23695 HOMO: -6.14161 LUMO: 1.80684 factor:1 | 1 (-0.78932) | -1 | -1 |
| G: -5312.08193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.24002 HOMO: -6.81373 LUMO: 1.91024 factor:1 | 1 (-0.79240) | -1 | -1 |
| G: -5312.08193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.05303 HOMO: -6.81917 LUMO: 2.34834 factor:1 | 1 (-0.60540) | -1 | -1 |
| G: -5312.08193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.00054 HOMO: -6.72121 LUMO: 1.90208 factor:1 | 1 (-0.55291) | -1 | -1 |
| G: -5312.08193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.78951 HOMO: -7.51851 LUMO: 0.26939 factor:1 | 1 (-0.34188) | -1 | -1 |
| G: -5312.08193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.03101 HOMO: -6.65318 LUMO: -0.57144 factor:1 | 1 (-0.58338) | -1 | -1 |
| G: -5312.08193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.20609 HOMO: -6.77564 LUMO: -0.72654 factor:1 | 1 (-0.75846) | -1 | -1 |
| G: -5312.08193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.03836 HOMO: -6.80557 LUMO: -0.60954 factor:1 | 1 (-0.59073) | -1 | -1 |
| G: -5312.08193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.91520 HOMO: -7.35524 LUMO: 0.27483 factor:1 | 1 (-0.46757) | -1 | -1 |
| G: -5312.08193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.18606 HOMO: -6.94979 LUMO: -0.83811 factor:1 | 1 (-0.73844) | -1 | -1 |
| G: -5312.08193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.73112 HOMO: -6.13345 LUMO: -0.67212 factor:1 | 1 (-0.28349) | -1 | -1 |
| G: -5312.08193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.61925 HOMO: -6.47359 LUMO: -0.59321 factor:1 | 1 (-0.17162) | -1 | -1 |
| G: -5312.08193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.08764 HOMO: -6.52257 LUMO: -0.54695 factor:1 | 1 (-0.64001) | -1 | -1 |
| G: -5312.08193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.22753 HOMO: -6.61781 LUMO: -0.69661 factor:1 | 1 (-0.77991) | -1 | -1 |
| G: -5312.08193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.01792 HOMO: -6.77564 LUMO: -0.80001 factor:1 | 1 (-0.57030) | -1 | -1 |
| G: -5312.08193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.30457 HOMO: -7.35252 LUMO: -1.00410 factor:1 | 1 (-0.85694) | -1 | -1 |
| G: -5312.08193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.11387 HOMO: -6.35386 LUMO: -0.38912 factor:1 | 1 (-0.66624) | -1 | -1 |
| G: -5312.08193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.87577 HOMO: -6.80285 LUMO: -0.52246 factor:1 | 1 (-0.42814) | -1 | -1 |
| G: -5312.08193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.67611 HOMO: -7.23279 LUMO: 0.30477 factor:1 | 1 (-1.22849) | -1 | -1 |
| G: -5312.08193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.67802 HOMO: -7.13483 LUMO: -0.76192 factor:1 | 1 (-1.23039) | -1 | -1 |
| G: -5312.08193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.99155 HOMO: -6.71849 LUMO: -0.48164 factor:1 | 1 (-1.54392) | -1 | -1 |
| G: -5312.08193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.90575 HOMO: -6.85455 LUMO: -0.69389 factor:1 | 1 (-1.45812) | -1 | -1 |
| G: -5312.08193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.85865 HOMO: -6.96339 LUMO: -0.73743 factor:1 | 1 (-1.41102) | -1 | -1 |
| G: -5312.08193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.81416 HOMO: -7.50490 LUMO: 0.28844 factor:1 | 1 (-1.36653) | -1 | -1 |
| G: -5312.08193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11578.01541 HOMO: -6.63958 LUMO: -0.50069 factor:1 | 1 (-1.56778) | -1 | -1 |
| G: -5312.08193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11578.09452 HOMO: -6.78924 LUMO: -0.69661 factor:1 | 1 (-1.64689) | -1 | -1 |
| G: -5312.08193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.90474 HOMO: -7.44776 LUMO: 0.33742 factor:1 | 1 (-1.45712) | -1 | -1 |
| G: -5312.08193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.85944 HOMO: -6.15249 LUMO: 0.66396 factor:1 | 1 (-1.41181) | -1 | -1 |
| G: -5312.08193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.87750 HOMO: -6.17426 LUMO: 0.55511 factor:1 | 1 (-1.42988) | -1 | -1 |
| G: -5312.08193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.94532 HOMO: -6.83550 LUMO: 0.28844 factor:1 | 1 (-1.49769) | -1 | -1 |
| G: -5312.08193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.53225 HOMO: -6.32393 LUMO: 0.47620 factor:1 | 1 (-1.08462) | -1 | -1 |
| G: -5312.08193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.52909 HOMO: -6.32937 LUMO: 0.45987 factor:1 | 1 (-1.08146) | -1 | -1 |
| G: -5312.08193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.18925 HOMO: -7.37429 LUMO: 0.09252 factor:1 | 1 (-0.74162) | -1 | -1 |
| G: -5312.08193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.09014 HOMO: -6.54434 LUMO: -0.39729 factor:1 | 1 (-0.64252) | -1 | -1 |
| G: -5312.08193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.02601 HOMO: -7.35524 LUMO: 0.28028 factor:1 | 1 (-0.57838) | -1 | -1 |
| G: -5312.08193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.12761 HOMO: -6.95523 LUMO: -0.86804 factor:1 | 1 (-0.67999) | -1 | -1 |
| G: -5312.08193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.23515 HOMO: -6.63958 LUMO: -0.65307 factor:1 | 1 (-0.78752) | -1 | -1 |
| G: -5312.08193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.42912 HOMO: -6.73482 LUMO: -0.67212 factor:1 | 1 (-0.98149) | -1 | -1 |
| G: -5312.08193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.25564 HOMO: -6.37835 LUMO: -0.53606 factor:1 | 1 (-0.80801) | -1 | -1 |
| G: -5312.08193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.07262 HOMO: -6.71849 LUMO: -0.61226 factor:1 | 1 (-0.62499) | -1 | -1 |
| G: -5312.08193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.96851 HOMO: -6.68584 LUMO: -1.11022 factor:1 | 1 (-0.52088) | -1 | -1 |
| G: -5312.08193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.64830 HOMO: -6.80285 LUMO: -0.79185 factor:1 | 1 (-1.20068) | -1 | -1 |
| G: -5312.08193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.78792 HOMO: -7.14571 LUMO: -0.94696 factor:1 | 1 (-1.34030) | -1 | -1 |
| G: -5312.08193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.77935 HOMO: -7.16204 LUMO: -0.66124 factor:1 | 1 (-1.33173) | -1 | -1 |
| G: -5312.08193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.48000 HOMO: -6.54978 LUMO: -0.54967 factor:1 | 1 (-1.03237) | -1 | -1 |
| G: -5312.08193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.60520 HOMO: -6.75114 LUMO: -0.70750 factor:1 | 1 (-1.15757) | -1 | -1 |
| G: -5312.08193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.52966 HOMO: -7.22190 LUMO: 0.39184 factor:1 | 1 (-1.08203) | -1 | -1 |
| G: -5312.08193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.73465 HOMO: -7.43959 LUMO: 0.30477 factor:1 | 1 (-1.28702) | -1 | -1 |
| G: -5312.08193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.79674 HOMO: -6.87360 LUMO: -0.77552 factor:1 | 1 (-1.34911) | -1 | -1 |
| G: -5312.08193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.89661 HOMO: -6.82734 LUMO: -0.59593 factor:1 | 1 (-1.44898) | -1 | -1 |
| G: -5312.08193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.76188 HOMO: -6.65318 LUMO: -0.46259 factor:1 | 1 (-1.31426) | -1 | -1 |
| G: -5312.08193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.63121 HOMO: -7.05863 LUMO: -1.17009 factor:1 | 1 (-1.18359) | -1 | -1 |
| G: -5312.08193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.66942 HOMO: -6.57427 LUMO: -0.48708 factor:1 | 1 (-1.22179) | -1 | -1 |
| G: -5312.08193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.44680 HOMO: -6.60420 LUMO: -0.38096 factor:1 | 1 (-0.99917) | -1 | -1 |
| G: -5312.08193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.38041 HOMO: -6.72121 LUMO: -0.66668 factor:1 | 1 (-0.93278) | -1 | -1 |
| G: -5312.08193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.87582 HOMO: -6.52257 LUMO: -0.19320 factor:1 | 1 (-1.42819) | -1 | -1 |
| G: -5312.08193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.78741 HOMO: -6.28039 LUMO: -0.27211 factor:1 | 1 (-1.33978) | -1 | -1 |
| G: -5312.08193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.57883 HOMO: -6.71849 LUMO: -0.42722 factor:1 | 1 (-1.13120) | -1 | -1 |
| G: -5312.08193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.53548 HOMO: -6.27495 LUMO: 0.27756 factor:1 | 1 (-1.08786) | -1 | -1 |
| G: -5312.08193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.71884 HOMO: -6.21780 LUMO: 0.46531 factor:1 | 1 (-1.27121) | -1 | -1 |
| G: -5312.08193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.56027 HOMO: -6.52257 LUMO: -0.64491 factor:1 | 1 (-1.11265) | -1 | -1 |
| G: -5312.08193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.60539 HOMO: -6.73754 LUMO: 1.83133 factor:1 | 1 (-1.15776) | -1 | -1 |
| G: -5312.08193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.86542 HOMO: -6.67223 LUMO: 1.88847 factor:1 | 1 (-1.41779) | -1 | -1 |
| G: -5312.08193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.84153 HOMO: -6.82189 LUMO: 1.59187 factor:1 | 1 (-1.39390) | -1 | -1 |
| G: -5312.08193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.79122 HOMO: -6.43277 LUMO: 1.76330 factor:1 | 1 (-1.34359) | -1 | -1 |
| G: -5312.08193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.86757 HOMO: -6.48175 LUMO: 1.77962 factor:1 | 1 (-1.41994) | -1 | -1 |
| G: -5312.08193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.44610 HOMO: -6.50352 LUMO: 1.68438 factor:1 | 1 (-0.99847) | -1 | -1 |
| G: -5312.08193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.48253 HOMO: -6.31576 LUMO: 2.03813 factor:1 | 1 (-1.03490) | -1 | -1 |
| G: -5312.08193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11578.00534 HOMO: -6.27495 LUMO: 1.99459 factor:1 | 1 (-1.55772) | -1 | -1 |
| G: -5312.08193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.02437 HOMO: -6.23957 LUMO: 2.17147 factor:1 | 1 (-0.57675) | -1 | -1 |
| G: -5312.08193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.83112 HOMO: -6.78108 LUMO: 2.16875 factor:1 | 1 (-0.38349) | -1 | -1 |
| G: -5312.08193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.03741 HOMO: -6.34297 LUMO: 2.10344 factor:1 | 1 (-0.58978) | -1 | -1 |
| G: -5312.08193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.16111 HOMO: -6.30216 LUMO: 2.00004 factor:1 | 1 (-0.71348) | -1 | -1 |
| G: -5312.08193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.77963 HOMO: -6.72665 LUMO: 2.09528 factor:1 | 1 (-0.33201) | -1 | -1 |
| G: -5312.08193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.97368 HOMO: -6.86543 LUMO: 1.91568 factor:1 | 1 (-0.52605) | -1 | -1 |
| G: -5312.08193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.91398 HOMO: -5.83956 LUMO: 1.89391 factor:1 | 1 (-0.46635) | -1 | -1 |
| G: -5312.08193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.86132 HOMO: -6.42189 LUMO: 2.03269 factor:1 | 1 (-0.41369) | -1 | -1 |
| G: -5312.08193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.74589 HOMO: -6.07630 LUMO: 1.80956 factor:1 | 1 (-0.29826) | -1 | -1 |
| G: -5312.08193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.68246 HOMO: -6.43277 LUMO: 1.81772 factor:1 | 1 (-0.23483) | -1 | -1 |
| G: -5312.08193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.05036 HOMO: -7.03959 LUMO: 1.78779 factor:1 | 1 (-0.60273) | -1 | -1 |
| G: -5312.08193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.90026 HOMO: -6.72121 LUMO: 2.29664 factor:1 | 1 (-0.45263) | -1 | -1 |
| G: -5312.08193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.29856 HOMO: -6.62869 LUMO: 2.04630 factor:1 | 1 (-0.85093) | -1 | -1 |
| G: -5312.08193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.01833 HOMO: -6.63958 LUMO: 1.84221 factor:1 | 1 (-0.57070) | -1 | -1 |
| G: -5312.08193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.92728 HOMO: -6.70761 LUMO: 1.67350 factor:1 | 1 (-0.47966) | -1 | -1 |
| G: -5312.08193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.89828 HOMO: -6.00283 LUMO: 1.64357 factor:1 | 1 (-0.45065) | -1 | -1 |
| G: -5312.08193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.85180 HOMO: -6.48719 LUMO: 1.70343 factor:1 | 1 (-0.40417) | -1 | -1 |
| G: -5312.08193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.98070 HOMO: -6.13345 LUMO: 1.44492 factor:1 | 1 (-0.53307) | -1 | -1 |
| G: -5312.08193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.20810 HOMO: -6.11168 LUMO: 1.70071 factor:1 | 1 (-0.76048) | -1 | -1 |
| G: -5312.08193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.69237 HOMO: -6.09535 LUMO: 1.82316 factor:1 | 1 (-0.24474) | -1 | -1 |
| G: -5312.08193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.96824 HOMO: -6.81101 LUMO: 1.63540 factor:1 | 1 (-0.52061) | -1 | -1 |
| G: -5312.08193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.09997 HOMO: -6.80013 LUMO: 2.12249 factor:1 | 1 (-0.65234) | -1 | -1 |
| G: -5312.08193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.91844 HOMO: -6.48447 LUMO: 1.94561 factor:1 | 1 (-0.47081) | -1 | -1 |
| G: -5312.08193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.90443 HOMO: -6.72393 LUMO: 2.06534 factor:1 | 1 (-0.45680) | -1 | -1 |
| G: -5312.08193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.82214 HOMO: -6.34570 LUMO: 1.98915 factor:1 | 1 (-0.37451) | -1 | -1 |
| G: -5312.08193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.06573 HOMO: -6.31304 LUMO: 1.87759 factor:1 | 1 (-0.61811) | -1 | -1 |
| G: -5312.08193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.81558 HOMO: -6.77564 LUMO: 1.81228 factor:1 | 1 (-0.36795) | -1 | -1 |
| G: -5312.08193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.76570 HOMO: -6.58516 LUMO: 2.34834 factor:1 | 1 (-0.31807) | -1 | -1 |
| G: -5312.08193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.68400 HOMO: -6.68040 LUMO: 2.20412 factor:1 | 1 (-1.23638) | -1 | -1 |
| G: -5312.08193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.88300 HOMO: -6.20964 LUMO: 2.17147 factor:1 | 1 (-1.43537) | -1 | -1 |
| G: -5312.08193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.80422 HOMO: -6.54706 LUMO: 2.03813 factor:1 | 1 (-1.35660) | -1 | -1 |
| G: -5312.08193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.33064 HOMO: -6.54162 LUMO: 2.17419 factor:1 | 1 (-0.88301) | -1 | -1 |
| G: -5312.08193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.75894 HOMO: -6.75659 LUMO: 2.22589 factor:1 | 1 (-1.31132) | -1 | -1 |
| G: -5312.08193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.47532 HOMO: -6.59604 LUMO: 2.59325 factor:1 | 1 (-1.02769) | -1 | -1 |
| G: -5312.08193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.45513 HOMO: -6.11712 LUMO: 2.02181 factor:1 | 1 (-1.00750) | -1 | -1 |
| G: -5312.08193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.65290 HOMO: -6.63141 LUMO: 2.09256 factor:1 | 1 (-1.20527) | -1 | -1 |
| G: -5312.08193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.93150 HOMO: -6.61781 LUMO: 1.86126 factor:1 | 1 (-0.48387) | -1 | -1 |
| G: -5312.08193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.92059 HOMO: -6.63958 LUMO: 1.77146 factor:1 | 1 (-0.47296) | -1 | -1 |
| G: -5312.08193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.20541 HOMO: -6.60420 LUMO: 1.54561 factor:1 | 1 (-0.75778) | -1 | -1 |
| G: -5312.08193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.73593 HOMO: -6.52529 LUMO: 2.05174 factor:1 | 1 (-0.28830) | -1 | -1 |
| G: -5312.08193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.74094 HOMO: -6.80285 LUMO: 2.13609 factor:1 | 1 (-0.29331) | -1 | -1 |
| G: -5312.08193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.04489 HOMO: -6.51168 LUMO: 2.25855 factor:1 | 1 (-0.59726) | -1 | -1 |
| G: -5312.08193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.92568 HOMO: -6.64774 LUMO: 2.46263 factor:1 | 1 (-0.47805) | -1 | -1 |
| G: -5312.08193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.98187 HOMO: -6.40828 LUMO: 1.99732 factor:1 | 1 (-0.53424) | -1 | -1 |
| G: -5312.08193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.27722 HOMO: -5.97562 LUMO: 1.56465 factor:1 | 1 (-0.82959) | -1 | -1 |
| G: -5312.08193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.82358 HOMO: -6.75659 LUMO: 2.23405 factor:1 | 1 (-0.37595) | -1 | -1 |
| G: -5312.08193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.57054 HOMO: -6.68584 LUMO: 2.09528 factor:1 | 1 (-0.12291) | -1 | -1 |
| G: -5312.08193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.08184 HOMO: -6.86543 LUMO: 1.95106 factor:1 | 1 (-0.63422) | -1 | -1 |
| G: -5312.08193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.70129 HOMO: -6.47359 LUMO: 1.82316 factor:1 | 1 (-0.25366) | -1 | -1 |
| G: -5312.08193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.94511 HOMO: -6.87632 LUMO: 2.08439 factor:1 | 1 (-0.49748) | -1 | -1 |
| G: -5312.08193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.06628 HOMO: -6.33753 LUMO: 2.16603 factor:1 | 1 (-0.61865) | -1 | -1 |
| G: -5312.08193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.78309 HOMO: -6.92258 LUMO: 1.72248 factor:1 | 1 (-0.33546) | -1 | -1 |
| G: -5312.08193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.83762 HOMO: -6.62597 LUMO: 2.10344 factor:1 | 1 (-0.38999) | -1 | -1 |
| G: -5312.08193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.66676 HOMO: -6.63141 LUMO: 1.94017 factor:1 | 1 (-0.21913) | -1 | -1 |
| G: -5312.08193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.03112 HOMO: -6.48447 LUMO: 1.91840 factor:1 | 1 (-0.58349) | -1 | -1 |
| G: -5312.08193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.22819 HOMO: -6.41372 LUMO: 1.61364 factor:1 | 1 (-0.78056) | -1 | -1 |
| G: -5312.08193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.85466 HOMO: -6.37291 LUMO: 1.79051 factor:1 | 1 (-0.40703) | -1 | -1 |
| G: -5312.08193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.01031 HOMO: -6.13073 LUMO: 1.77962 factor:1 | 1 (-0.56268) | -1 | -1 |
| G: -5312.08193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.97088 HOMO: -6.13073 LUMO: 1.98915 factor:1 | 1 (-0.52325) | -1 | -1 |
| G: -5312.08193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.19308 HOMO: -6.44094 LUMO: 1.58370 factor:1 | 1 (-0.74546) | -1 | -1 |
| G: -5312.08193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.08269 HOMO: -6.87087 LUMO: -0.82995 factor:1 | 1 (-0.63506) | -1 | -1 |
| G: -5312.08193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.92135 HOMO: -6.67223 LUMO: 1.08029 factor:1 | 1 (-0.47372) | -1 | -1 |
| G: -5312.08193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.92456 HOMO: -6.82462 LUMO: 0.91702 factor:1 | 1 (-0.47693) | -1 | -1 |
| G: -5312.08193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.84701 HOMO: -6.65863 LUMO: 1.52656 factor:1 | 1 (-0.39938) | -1 | -1 |
| G: -5312.08193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.89330 HOMO: -6.78924 LUMO: 0.86260 factor:1 | 1 (-0.44567) | -1 | -1 |
| G: -5312.08193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.72197 HOMO: -6.68584 LUMO: 0.94424 factor:1 | 1 (-0.27435) | -1 | -1 |
| G: -5312.08193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.94451 HOMO: -6.58788 LUMO: 1.00138 factor:1 | 1 (-0.49688) | -1 | -1 |
| G: -5312.08193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.79626 HOMO: -6.79740 LUMO: 0.91430 factor:1 | 1 (-0.34863) | -1 | -1 |
| G: -5312.08193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.07939 HOMO: -6.67223 LUMO: 0.80274 factor:1 | 1 (-0.63177) | -1 | -1 |
| G: -5312.08193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.96478 HOMO: -6.95251 LUMO: 0.90614 factor:1 | 1 (-0.51715) | -1 | -1 |
| G: -5312.08193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.76636 HOMO: -7.19469 LUMO: 1.34152 factor:1 | 1 (-0.31873) | -1 | -1 |
| G: -5312.08193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.13714 HOMO: -6.59332 LUMO: -0.76464 factor:1 | 1 (-0.68951) | -1 | -1 |
| G: -5312.08193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.75381 HOMO: -6.77564 LUMO: -0.90886 factor:1 | 1 (-0.30618) | -1 | -1 |
| G: -5312.08193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.68619 HOMO: -6.57971 LUMO: -0.41633 factor:1 | 1 (-0.23856) | -1 | -1 |
| G: -5312.08193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.49944 HOMO: -6.68856 LUMO: -0.58232 factor:1 | 1 (-0.05181) | -1 | -1 |
| G: -5312.08193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.92116 HOMO: -6.87087 LUMO: -0.71022 factor:1 | 1 (-0.47353) | -1 | -1 |
| G: -5312.08193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.03504 HOMO: -6.67767 LUMO: -0.74559 factor:1 | 1 (-0.58741) | -1 | -1 |
| G: -5312.08193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.07667 HOMO: -6.68040 LUMO: -0.65307 factor:1 | 1 (-0.62905) | -1 | -1 |
| G: -5312.08193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.74293 HOMO: -6.32937 LUMO: 0.80274 factor:1 | 1 (-0.29530) | -1 | -1 |
| G: -5312.08193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.64899 HOMO: -6.29671 LUMO: 0.82723 factor:1 | 1 (-0.20136) | -1 | -1 |
| G: -5312.08193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.11213 HOMO: -6.67767 LUMO: 0.59321 factor:1 | 1 (-0.66450) | -1 | -1 |
| G: -5312.08193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.13232 HOMO: -6.77836 LUMO: 0.50341 factor:1 | 1 (-0.68469) | -1 | -1 |
| G: -5312.08193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.21714 HOMO: -6.61781 LUMO: 0.42450 factor:1 | 1 (-0.76951) | -1 | -1 |
| G: -5312.08193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.27488 HOMO: -6.83278 LUMO: 0.39457 factor:1 | 1 (-0.82725) | -1 | -1 |
| G: -5312.08193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.01229 HOMO: -6.56883 LUMO: 0.64219 factor:1 | 1 (-0.56466) | -1 | -1 |
| G: -5312.08193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.12990 HOMO: -6.71577 LUMO: 0.40001 factor:1 | 1 (-0.68227) | -1 | -1 |
| G: -5312.08193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.98062 HOMO: -6.86543 LUMO: -0.74287 factor:1 | 1 (-0.53299) | -1 | -1 |
| G: -5312.08193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.63745 HOMO: -6.68584 LUMO: -0.69389 factor:1 | 1 (-1.18982) | -1 | -1 |
| G: -5312.08193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.52874 HOMO: -6.61237 LUMO: -0.48980 factor:1 | 1 (-1.08111) | -1 | -1 |
| G: -5312.08193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.70515 HOMO: -6.80285 LUMO: -0.58232 factor:1 | 1 (-1.25752) | -1 | -1 |
| G: -5312.08193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.89748 HOMO: -6.88992 LUMO: -0.70205 factor:1 | 1 (-1.44985) | -1 | -1 |
| G: -5312.08193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.57842 HOMO: -6.95251 LUMO: -0.71838 factor:1 | 1 (-1.13080) | -1 | -1 |
| G: -5312.08193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.45472 HOMO: -7.52123 LUMO: 0.27211 factor:1 | 1 (-1.00709) | -1 | -1 |
| G: -5312.08193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.96644 HOMO: -6.76747 LUMO: -0.74015 factor:1 | 1 (-0.51881) | -1 | -1 |
| G: -5312.08193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.98712 HOMO: -6.55250 LUMO: -0.49797 factor:1 | 1 (-0.53949) | -1 | -1 |
| G: -5312.08193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.79120 HOMO: -6.50896 LUMO: -0.46804 factor:1 | 1 (-0.34357) | -1 | -1 |
| G: -5312.08193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.68412 HOMO: -7.45320 LUMO: 0.08436 factor:1 | 1 (-0.23649) | -1 | -1 |
| G: -5312.08193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.41359 HOMO: -6.82462 LUMO: -0.70477 factor:1 | -1 (0.03404) | -1 | -1 |
| G: -5312.08193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.86970 HOMO: -6.57155 LUMO: -0.43538 factor:1 | 1 (-0.42208) | -1 | -1 |
| G: -5312.08193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.60431 HOMO: -6.72665 LUMO: -0.55239 factor:1 | 1 (-0.15668) | -1 | -1 |
| G: -5312.08193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.29957 HOMO: -7.05319 LUMO: -1.08573 factor:1 | -1 (0.14806) | -1 | -1 |
| G: -5312.08193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.16326 HOMO: -6.56067 LUMO: -0.45715 factor:1 | 1 (-0.71563) | -1 | -1 |
| G: -5312.08193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.08745 HOMO: -6.76475 LUMO: -0.53879 factor:1 | 1 (-0.63982) | -1 | -1 |
| G: -5312.08193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.26451 HOMO: -6.67223 LUMO: -0.45987 factor:1 | 1 (-0.81689) | -1 | -1 |
| G: -5312.08193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.38332 HOMO: -6.44094 LUMO: -0.72110 factor:1 | 1 (-0.93569) | -1 | -1 |
| G: -5312.08193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.39948 HOMO: -6.66951 LUMO: -0.67756 factor:1 | 1 (-0.95185) | -1 | -1 |
| G: -5312.08193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.03632 HOMO: -6.69400 LUMO: -0.62858 factor:1 | 1 (-0.58869) | -1 | -1 |
| G: -5312.08193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.09812 HOMO: -6.51985 LUMO: -0.37007 factor:1 | 1 (-0.65049) | -1 | -1 |
| G: -5312.08193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.94685 HOMO: -5.98378 LUMO: 0.78641 factor:1 | 1 (-0.49922) | -1 | -1 |
| G: -5312.08193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.28601 HOMO: -6.11440 LUMO: 0.71294 factor:1 | 1 (-0.83838) | -1 | -1 |
| G: -5312.08193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.99713 HOMO: -6.45182 LUMO: 0.63947 factor:1 | 1 (-0.54951) | -1 | -1 |
| G: -5312.08193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.09074 HOMO: -6.78924 LUMO: 0.37007 factor:1 | 1 (-0.64311) | -1 | -1 |
| G: -5312.08193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.34656 HOMO: -6.63686 LUMO: 0.54423 factor:1 | 1 (-0.89893) | -1 | -1 |
| G: -5312.08193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.19115 HOMO: -6.66679 LUMO: 0.48708 factor:1 | 1 (-0.74352) | -1 | -1 |
| G: -5312.08193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.84086 HOMO: -6.81917 LUMO: 0.31021 factor:1 | 1 (-0.39323) | -1 | -1 |
| G: -5312.08193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.68709 HOMO: -6.28583 LUMO: 0.44899 factor:1 | 1 (-0.23946) | -1 | -1 |
| G: -5312.08193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.80132 HOMO: -6.61237 LUMO: 0.49525 factor:1 | 1 (-0.35369) | -1 | -1 |
| G: -5312.08193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.69625 HOMO: -7.08857 LUMO: 0.38368 factor:1 | 1 (-1.24862) | -1 | -1 |
| G: -5312.08193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.81827 HOMO: -6.53890 LUMO: -0.68845 factor:1 | 1 (-1.37064) | -1 | -1 |
| G: -5312.08193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.88526 HOMO: -6.56611 LUMO: -0.66396 factor:1 | 1 (-1.43763) | -1 | -1 |
| G: -5312.08193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.88980 HOMO: -6.04909 LUMO: -0.59865 factor:1 | 1 (-1.44218) | -1 | -1 |
| G: -5312.08193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11578.06652 HOMO: -6.74842 LUMO: -0.77825 factor:1 | 1 (-1.61889) | -1 | -1 |
| G: -5312.08193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.83829 HOMO: -6.82462 LUMO: -0.61498 factor:1 | 1 (-1.39067) | -1 | -1 |
| G: -5312.08193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.65535 HOMO: -7.40694 LUMO: 0.32926 factor:1 | 1 (-1.20772) | -1 | -1 |
| G: -5312.08193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.04835 HOMO: -6.80557 LUMO: -0.57416 factor:1 | 1 (-0.60072) | -1 | -1 |
| G: -5312.08193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.15640 HOMO: -6.76747 LUMO: -0.67484 factor:1 | 1 (-0.70877) | -1 | -1 |
| G: -5312.08193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.17488 HOMO: -7.23279 LUMO: 0.48980 factor:1 | 1 (-0.72725) | -1 | -1 |
| G: -5312.08193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.31189 HOMO: -6.62869 LUMO: -0.24762 factor:1 | 1 (-0.86426) | -1 | -1 |
| G: -5312.08193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.35012 HOMO: -6.65863 LUMO: -0.28028 factor:1 | 1 (-0.90249) | -1 | -1 |
| G: -5312.08193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.09091 HOMO: -6.50352 LUMO: -0.44899 factor:1 | 1 (-0.64328) | -1 | -1 |
| G: -5312.08193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.99406 HOMO: -6.62053 LUMO: -0.88437 factor:1 | 1 (-0.54643) | -1 | -1 |
| G: -5312.08193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.75104 HOMO: -6.73754 LUMO: -0.77825 factor:1 | 1 (-0.30341) | -1 | -1 |
| G: -5312.08193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.06114 HOMO: -7.24639 LUMO: 0.35647 factor:1 | 1 (-0.61351) | -1 | -1 |
| G: -5312.08193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.94192 HOMO: -6.46270 LUMO: -0.48164 factor:1 | 1 (-0.49429) | -1 | -1 |
| G: -5312.08193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.88837 HOMO: -6.14161 LUMO: -0.66396 factor:1 | 1 (-0.44074) | -1 | -1 |
| G: -5312.08193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.07659 HOMO: -6.63414 LUMO: 1.51295 factor:1 | 1 (-0.62896) | -1 | -1 |
| G: -5312.08193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.91991 HOMO: -6.52529 LUMO: 1.65989 factor:1 | 1 (-0.47228) | -1 | -1 |
| G: -5312.08193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.06304 HOMO: -6.63686 LUMO: 1.64629 factor:1 | 1 (-0.61541) | -1 | -1 |
| G: -5312.08193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.96138 HOMO: -6.49808 LUMO: 1.60003 factor:1 | 1 (-0.51375) | -1 | -1 |
| G: -5312.08193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.70750 HOMO: -6.85183 LUMO: 1.96194 factor:1 | 1 (-0.25987) | -1 | -1 |
| G: -5312.08193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.84739 HOMO: -6.90081 LUMO: 1.82316 factor:1 | 1 (-0.39976) | -1 | -1 |
| G: -5312.08193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.58676 HOMO: -6.20147 LUMO: 1.95106 factor:1 | 1 (-0.13913) | -1 | -1 |
| G: -5312.08193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.81666 HOMO: -7.05047 LUMO: 1.94289 factor:1 | 1 (-1.36903) | -1 | -1 |
| G: -5312.08193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.73437 HOMO: -6.11440 LUMO: 1.83949 factor:1 | 1 (-1.28674) | -1 | -1 |
| G: -5312.08193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.79914 HOMO: -6.65046 LUMO: 1.59187 factor:1 | 1 (-1.35151) | -1 | -1 |
| G: -5312.08193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.63399 HOMO: -6.81917 LUMO: 2.41365 factor:1 | 1 (-1.18636) | -1 | -1 |
| G: -5312.08193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.89179 HOMO: -6.40284 LUMO: 2.48984 factor:1 | 1 (-1.44416) | -1 | -1 |
| G: -5312.08193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.87125 HOMO: -7.04775 LUMO: 2.31025 factor:1 | 1 (-1.42362) | -1 | -1 |
| G: -5312.08193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11578.06064 HOMO: -6.64774 LUMO: 2.20140 factor:1 | 1 (-1.61301) | -1 | -1 |
| G: -5312.08193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.61208 HOMO: -6.72393 LUMO: 2.28304 factor:1 | 1 (-1.16446) | -1 | -1 |
| G: -5312.08193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.62373 HOMO: -6.35114 LUMO: 1.84765 factor:1 | 1 (-1.17610) | -1 | -1 |
| G: -5312.08193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.53227 HOMO: -6.41100 LUMO: 1.74697 factor:1 | 1 (-1.08465) | -1 | -1 |
| G: -5312.08193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.94232 HOMO: -6.34297 LUMO: 1.55921 factor:1 | 1 (-1.49469) | -1 | -1 |
| G: -5312.08193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.12125 HOMO: -6.31848 LUMO: 1.67622 factor:1 | 1 (-0.67362) | -1 | -1 |
| G: -5312.08193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.03354 HOMO: -6.50896 LUMO: 2.02725 factor:1 | 1 (-0.58592) | -1 | -1 |
| G: -5312.08193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.34838 HOMO: -6.28583 LUMO: 2.00548 factor:1 | 1 (-0.90075) | -1 | -1 |
| G: -5312.08193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.90081 HOMO: -6.67495 LUMO: 1.92384 factor:1 | 1 (-0.45318) | -1 | -1 |
| G: -5312.08193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.73860 HOMO: -6.17154 LUMO: 2.39732 factor:1 | 1 (-0.29097) | -1 | -1 |
| G: -5312.08193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.93972 HOMO: -6.84911 LUMO: 2.24766 factor:1 | 1 (-0.49209) | -1 | -1 |
| G: -5312.08193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.95477 HOMO: -6.77564 LUMO: 2.38372 factor:1 | 1 (-0.50714) | -1 | -1 |
| G: -5312.08193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.23238 HOMO: -6.18243 LUMO: 2.40821 factor:1 | 1 (-0.78475) | -1 | -1 |
| G: -5312.08193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.09940 HOMO: -6.40828 LUMO: 2.22589 factor:1 | 1 (-0.65177) | -1 | -1 |
| G: -5312.08193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.70935 HOMO: -6.74570 LUMO: 1.88303 factor:1 | 1 (-0.26172) | -1 | -1 |
| G: -5312.08193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.63765 HOMO: -6.29944 LUMO: 2.05174 factor:1 | 1 (-0.19002) | -1 | -1 |
| G: -5312.08193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.10530 HOMO: -7.00693 LUMO: 2.16331 factor:1 | 1 (-0.65767) | -1 | -1 |
| G: -5312.08193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.99441 HOMO: -6.89537 LUMO: 2.19596 factor:1 | 1 (-0.54679) | -1 | -1 |
| G: -5312.08193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.93267 HOMO: -6.72665 LUMO: 2.03813 factor:1 | 1 (-0.48504) | -1 | -1 |
| G: -5312.08193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.20152 HOMO: -6.69944 LUMO: 2.36467 factor:1 | 1 (-0.75389) | -1 | -1 |
| G: -5312.08193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.25621 HOMO: -6.92802 LUMO: 1.72792 factor:1 | 1 (-0.80859) | -1 | -1 |
| G: -5312.08193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.79329 HOMO: -6.12256 LUMO: 1.85310 factor:1 | 1 (-0.34567) | -1 | -1 |
| G: -5312.08193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.80742 HOMO: -6.70489 LUMO: 2.20956 factor:1 | 1 (-0.35979) | -1 | -1 |
| G: -5312.08193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.01920 HOMO: -6.94707 LUMO: 1.81500 factor:1 | 1 (-0.57158) | -1 | -1 |
| G: -5312.08193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.68891 HOMO: -6.39468 LUMO: 1.79051 factor:1 | 1 (-0.24128) | -1 | -1 |
| G: -5312.08193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.49084 HOMO: -6.69128 LUMO: 2.03813 factor:1 | 1 (-0.04321) | -1 | -1 |
| G: -5312.08193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.67669 HOMO: -6.55250 LUMO: 2.00548 factor:1 | 1 (-0.22907) | -1 | -1 |
| G: -5312.08193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.59922 HOMO: -6.24773 LUMO: 2.09256 factor:1 | 1 (-0.15159) | -1 | -1 |
| G: -5312.08193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.93433 HOMO: -6.85727 LUMO: 1.70071 factor:1 | 1 (-0.48670) | -1 | -1 |
| G: -5312.08193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.64290 HOMO: -6.71305 LUMO: 1.72520 factor:1 | 1 (-0.19527) | -1 | -1 |
| G: -5312.08193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.13787 HOMO: -6.81101 LUMO: 2.15514 factor:1 | 1 (-0.69024) | -1 | -1 |
| G: -5312.08193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.85610 HOMO: -6.93618 LUMO: 1.75513 factor:1 | 1 (-0.40847) | -1 | -1 |
| G: -5312.08193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.02211 HOMO: -6.63686 LUMO: 2.09800 factor:1 | 1 (-0.57449) | -1 | -1 |
| G: -5312.08193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.09765 HOMO: -6.98244 LUMO: 1.72520 factor:1 | 1 (-0.65003) | -1 | -1 |
| G: -5312.08193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.72420 HOMO: -6.37019 LUMO: 2.35923 factor:1 | 1 (-0.27658) | -1 | -1 |
| G: -5312.08193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.97920 HOMO: -6.55794 LUMO: 2.12521 factor:1 | 1 (-0.53157) | -1 | -1 |
| G: -5312.08193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.78480 HOMO: -6.45998 LUMO: 1.93201 factor:1 | 1 (-0.33718) | -1 | -1 |
| G: -5312.08193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.86992 HOMO: -6.71033 LUMO: 1.58370 factor:1 | 1 (-0.42229) | -1 | -1 |
| G: -5312.08193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.14786 HOMO: -6.67223 LUMO: 1.52928 factor:1 | 1 (-0.70023) | -1 | -1 |
| G: -5312.08193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.73572 HOMO: -6.72121 LUMO: 1.33608 factor:1 | 1 (-0.28809) | -1 | -1 |
| G: -5312.08193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.45800 HOMO: -6.89264 LUMO: 2.08983 factor:1 | 1 (-0.01037) | -1 | -1 |
| G: -5312.08193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.77854 HOMO: -6.31032 LUMO: 2.24766 factor:1 | 1 (-1.33091) | -1 | -1 |
| G: -5312.08193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.95933 HOMO: -6.79740 LUMO: 2.09528 factor:1 | 1 (-1.51170) | -1 | -1 |
| G: -5312.08193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.75620 HOMO: -6.78108 LUMO: 2.15786 factor:1 | 1 (-1.30857) | -1 | -1 |
| G: -5312.08193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.81748 HOMO: -6.50896 LUMO: 2.15786 factor:1 | 1 (-1.36985) | -1 | -1 |
| G: -5312.08193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.87786 HOMO: -6.56067 LUMO: 2.24494 factor:1 | 1 (-1.43023) | -1 | -1 |
| G: -5312.08193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11578.09582 HOMO: -6.72938 LUMO: 2.24494 factor:1 | 1 (-1.64819) | -1 | -1 |
| G: -5312.08193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11578.06219 HOMO: -6.40556 LUMO: 1.58642 factor:1 | 1 (-1.61456) | -1 | -1 |
| G: -5312.08193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.79258 HOMO: -6.63141 LUMO: 1.66262 factor:1 | 1 (-1.34495) | -1 | -1 |
| G: -5312.08193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.97930 HOMO: -6.97156 LUMO: 2.23678 factor:1 | 1 (-1.53167) | -1 | -1 |
| G: -5312.08193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.65464 HOMO: -6.86271 LUMO: 1.91296 factor:1 | 1 (-1.20702) | -1 | -1 |
| G: -5312.08193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.59236 HOMO: -6.50624 LUMO: 1.89119 factor:1 | 1 (-1.14473) | -1 | -1 |
| G: -5312.08193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.58583 HOMO: -6.70761 LUMO: 1.56193 factor:1 | 1 (-1.13820) | -1 | -1 |
| G: -5312.08193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.70866 HOMO: -6.60420 LUMO: 1.79595 factor:1 | 1 (-1.26103) | -1 | -1 |
| G: -5312.08193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.61007 HOMO: -6.85727 LUMO: 2.26943 factor:1 | 1 (-1.16244) | -1 | -1 |
| G: -5312.08193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.45736 HOMO: -6.23413 LUMO: 1.91024 factor:1 | 1 (-1.00973) | -1 | -1 |
| G: -5312.08193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.84159 HOMO: -6.84366 LUMO: 2.01364 factor:1 | 1 (-1.39396) | -1 | -1 |
| G: -5312.08193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.73775 HOMO: -6.63414 LUMO: 2.54971 factor:1 | 1 (-1.29012) | -1 | -1 |
| G: -5312.08193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.76866 HOMO: -6.52257 LUMO: 2.42998 factor:1 | 1 (-1.32103) | -1 | -1 |
| G: -5312.08193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.69198 HOMO: -6.61509 LUMO: 2.31297 factor:1 | 1 (-1.24435) | -1 | -1 |
| G: -5312.08193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.64398 HOMO: -6.45998 LUMO: 2.23405 factor:1 | 1 (-1.19635) | -1 | -1 |
| G: -5312.08193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.45382 HOMO: -6.86271 LUMO: 2.22317 factor:1 | 1 (-1.00620) | -1 | -1 |
| G: -5312.08193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.45067 HOMO: -6.84366 LUMO: 2.11432 factor:1 | 1 (-1.00304) | -1 | -1 |
| G: -5312.08193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.73813 HOMO: -6.85999 LUMO: 2.44902 factor:1 | 1 (-1.29050) | -1 | -1 |
| G: -5312.08193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.61706 HOMO: -6.73482 LUMO: 1.93745 factor:1 | 1 (-1.16944) | -1 | -1 |
| G: -5312.08193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.77612 HOMO: -6.91441 LUMO: 2.32385 factor:1 | 1 (-1.32849) | -1 | -1 |
| G: -5312.08193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.90036 HOMO: -6.16066 LUMO: 2.26399 factor:1 | 1 (-1.45273) | -1 | -1 |
| G: -5312.08193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.63804 HOMO: -6.71305 LUMO: 2.38644 factor:1 | 1 (-1.19042) | -1 | -1 |
| G: -5312.08193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.69415 HOMO: -7.08312 LUMO: 2.01636 factor:1 | 1 (-1.24653) | 1 | 1 |
| G: -5312.08193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.90746 HOMO: -6.15249 LUMO: 1.90752 factor:1 | 1 (-1.45984) | -1 | -1 |
| G: -5312.08193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.72390 HOMO: -6.83006 LUMO: 2.25855 factor:1 | 1 (-1.27627) | -1 | -1 |
| G: -5312.08193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.56887 HOMO: -6.77836 LUMO: 2.24766 factor:1 | 1 (-1.12125) | -1 | -1 |
| G: -5312.08193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.67791 HOMO: -6.66951 LUMO: 2.35923 factor:1 | 1 (-1.23028) | -1 | -1 |
| G: -5312.08193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.82305 HOMO: -6.68312 LUMO: 2.30208 factor:1 | 1 (-1.37543) | -1 | -1 |
| G: -5312.08193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.67788 HOMO: -6.49808 LUMO: 2.49801 factor:1 | 1 (-1.23025) | -1 | -1 |
| G: -5312.08193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.51148 HOMO: -6.62325 LUMO: 1.89935 factor:1 | 1 (-1.06386) | -1 | -1 |
| G: -5312.08193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.85220 HOMO: -6.80829 LUMO: 1.91296 factor:1 | 1 (-1.40457) | -1 | -1 |
| G: -5312.08193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.90191 HOMO: -6.64230 LUMO: 2.13065 factor:1 | 1 (-1.45429) | -1 | -1 |
| G: -5312.08193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.75690 HOMO: -6.40556 LUMO: 1.83949 factor:1 | 1 (-1.30928) | -1 | -1 |
| G: -5312.08193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.96763 HOMO: -6.48175 LUMO: 1.72248 factor:1 | 1 (-1.52000) | -1 | -1 |
| G: -5312.08193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.71554 HOMO: -6.61781 LUMO: 2.11432 factor:1 | 1 (-1.26791) | -1 | -1 |
| G: -5312.08193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.29466 HOMO: -6.34570 LUMO: 2.22317 factor:1 | 1 (-0.84704) | -1 | -1 |
| G: -5312.08193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.44297 HOMO: -7.00149 LUMO: 1.80139 factor:1 | 1 (-0.99534) | -1 | -1 |
| G: -5312.08193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.58400 HOMO: -6.66951 LUMO: 2.13065 factor:1 | 1 (-1.13637) | -1 | -1 |
| G: -5312.08193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.84418 HOMO: -6.54434 LUMO: 2.20140 factor:1 | 1 (-0.39655) | -1 | -1 |
| G: -5312.08193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.94143 HOMO: -6.67767 LUMO: 2.02997 factor:1 | 1 (-0.49381) | -1 | -1 |
| G: -5312.08193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.01006 HOMO: -6.49536 LUMO: 2.42998 factor:1 | 1 (-0.56243) | -1 | -1 |
| G: -5312.08193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.90769 HOMO: -6.70761 LUMO: 2.71025 factor:1 | 1 (-0.46006) | -1 | -1 |
| G: -5312.08193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.05496 HOMO: -6.62869 LUMO: 2.11160 factor:1 | 1 (-0.60733) | -1 | -1 |
| G: -5312.08193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.99221 HOMO: -6.61781 LUMO: 2.24494 factor:1 | 1 (-0.54458) | -1 | -1 |
| G: -5312.08193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.17472 HOMO: -6.66135 LUMO: 2.20956 factor:1 | 1 (-0.72709) | -1 | -1 |
| G: -5312.08193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.13744 HOMO: -6.95523 LUMO: 2.03813 factor:1 | 1 (-0.68981) | -1 | -1 |
| G: -5312.08193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.99251 HOMO: -7.11578 LUMO: 2.41365 factor:1 | 1 (-0.54488) | 1 | 1 |
| G: -5312.08193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.84116 HOMO: -6.99061 LUMO: 2.13881 factor:1 | 1 (-0.39353) | -1 | -1 |
| G: -5312.08193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.16936 HOMO: -6.43277 LUMO: 2.01364 factor:1 | 1 (-0.72173) | -1 | -1 |
| G: -5312.08193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.78358 HOMO: -6.79196 LUMO: 2.04358 factor:1 | 1 (-0.33595) | -1 | -1 |
| G: -5312.08193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.80780 HOMO: -7.08584 LUMO: 1.99732 factor:1 | 1 (-0.36017) | 1 | 1 |
| G: -5312.08193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.70978 HOMO: -6.46815 LUMO: 2.29936 factor:1 | 1 (-0.26215) | -1 | -1 |
| G: -5312.08193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.79713 HOMO: -6.78108 LUMO: 1.93745 factor:1 | 1 (-0.34950) | -1 | -1 |
| G: -5312.08193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.78929 HOMO: -6.43277 LUMO: 1.80956 factor:1 | 1 (-0.34167) | -1 | -1 |
| G: -5312.08193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.94217 HOMO: -6.71577 LUMO: -0.81090 factor:1 | 1 (-0.49454) | -1 | -1 |
| G: -5312.08193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.12008 HOMO: -7.14027 LUMO: -0.68028 factor:1 | 1 (-0.67245) | -1 | -1 |
| G: -5312.08193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.01882 HOMO: -7.03414 LUMO: -0.69661 factor:1 | 1 (-0.57119) | -1 | -1 |
| G: -5312.08193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.95409 HOMO: -6.64502 LUMO: -0.47348 factor:1 | 1 (-0.50646) | -1 | -1 |
| G: -5312.08193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.79112 HOMO: -6.60692 LUMO: 2.12793 factor:1 | 1 (-0.34349) | -1 | -1 |
| G: -5312.08193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.77260 HOMO: -6.66407 LUMO: 1.94561 factor:1 | 1 (-1.32498) | -1 | -1 |
| G: -5312.08193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.95446 HOMO: -7.10217 LUMO: 1.92384 factor:1 | 1 (-1.50683) | 1 | 1 |
| G: -5312.08193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.84308 HOMO: -6.84094 LUMO: 1.66534 factor:1 | 1 (-1.39545) | -1 | -1 |
| G: -5312.08193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.64814 HOMO: -6.93618 LUMO: 2.13065 factor:1 | 1 (-1.20051) | -1 | -1 |
| G: -5312.08193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.96434 HOMO: -6.60692 LUMO: 2.20684 factor:1 | 1 (-1.51671) | -1 | -1 |
| G: -5312.08193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.87887 HOMO: -6.85727 LUMO: 2.19324 factor:1 | 1 (-1.43124) | -1 | -1 |
| G: -5312.08193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11578.05479 HOMO: -6.31032 LUMO: 1.76330 factor:1 | 1 (-1.60716) | -1 | -1 |
| G: -5312.08193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.74382 HOMO: -6.43821 LUMO: 2.10072 factor:1 | 1 (-1.29619) | -1 | -1 |
| G: -5312.08193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.70240 HOMO: -6.42189 LUMO: 2.19596 factor:1 | 1 (-1.25477) | -1 | -1 |
| G: -5312.08193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11578.05517 HOMO: -6.40556 LUMO: 2.02181 factor:1 | 1 (-1.60754) | -1 | -1 |
| G: -5312.08193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.78167 HOMO: -6.41372 LUMO: 2.26671 factor:1 | 1 (-1.33404) | -1 | -1 |
| G: -5312.08193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.89421 HOMO: -6.60692 LUMO: 2.09800 factor:1 | 1 (-1.44658) | -1 | -1 |
| G: -5312.08193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.70341 HOMO: -6.75931 LUMO: 1.76602 factor:1 | 1 (-1.25578) | -1 | -1 |
| G: -5312.08193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.61546 HOMO: -6.39195 LUMO: 1.84221 factor:1 | 1 (-1.16783) | -1 | -1 |
| G: -5312.08193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.47061 HOMO: -6.74570 LUMO: 2.04085 factor:1 | 1 (-1.02298) | -1 | -1 |
| G: -5312.08193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.86670 HOMO: -6.77019 LUMO: 2.16875 factor:1 | 1 (-1.41907) | -1 | -1 |
| G: -5312.08193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.66833 HOMO: -6.15522 LUMO: 1.81772 factor:1 | 1 (-1.22070) | -1 | -1 |
| G: -5312.08193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.47921 HOMO: -6.48175 LUMO: 2.02453 factor:1 | 1 (-1.03158) | -1 | -1 |
| G: -5312.08193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.68082 HOMO: -6.57427 LUMO: 1.77962 factor:1 | 1 (-1.23319) | -1 | -1 |
| G: -5312.08193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.72773 HOMO: -6.57699 LUMO: 2.42998 factor:1 | 1 (-1.28011) | -1 | -1 |
| G: -5312.08193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.64346 HOMO: -6.35386 LUMO: 2.25310 factor:1 | 1 (-1.19583) | -1 | -1 |
| G: -5312.08193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.81846 HOMO: -6.80013 LUMO: 2.11160 factor:1 | 1 (-1.37083) | -1 | -1 |
| G: -5312.08193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.85870 HOMO: -6.24229 LUMO: 2.05718 factor:1 | 1 (-1.41107) | -1 | -1 |
| G: -5312.08193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.66534 HOMO: -6.42733 LUMO: 1.76874 factor:1 | 1 (-1.21771) | -1 | -1 |
| G: -5312.08193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.54071 HOMO: -6.56883 LUMO: 2.36195 factor:1 | 1 (-1.09308) | -1 | -1 |
| G: -5312.08193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.36441 HOMO: -6.72665 LUMO: 2.28848 factor:1 | 1 (-0.91678) | -1 | -1 |
| G: -5312.08193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.77329 HOMO: -6.39195 LUMO: 1.79051 factor:1 | 1 (-1.32566) | -1 | -1 |
| G: -5312.08193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.58389 HOMO: -6.70761 LUMO: 0.15510 factor:1 | 1 (-1.13627) | -1 | -1 |
| G: -5312.08193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.74156 HOMO: -6.44366 LUMO: -0.16871 factor:1 | 1 (-1.29393) | -1 | -1 |
| G: -5312.08193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.42620 HOMO: -6.68584 LUMO: 1.69527 factor:1 | 1 (-0.97858) | -1 | -1 |
| G: -5312.08193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.33679 HOMO: -6.26950 LUMO: 1.61636 factor:1 | 1 (-0.88916) | -1 | -1 |
| G: -5312.08193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.57853 HOMO: -6.47631 LUMO: 1.98915 factor:1 | 1 (-1.13091) | -1 | -1 |
| G: -5312.08193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.45037 HOMO: -6.58243 LUMO: 1.97283 factor:1 | 1 (-1.00274) | -1 | -1 |
| G: -5312.08193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.77092 HOMO: -6.51713 LUMO: 1.97283 factor:1 | 1 (-1.32329) | -1 | -1 |
| G: -5312.08193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.41891 HOMO: -6.65046 LUMO: 1.69255 factor:1 | 1 (-0.97128) | -1 | -1 |
| G: -5312.08193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.15923 HOMO: -6.26406 LUMO: 2.21773 factor:1 | 1 (-0.71160) | -1 | -1 |
| G: -5312.08193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.44599 HOMO: -6.88992 LUMO: 2.28304 factor:1 | 1 (-0.99836) | -1 | -1 |
| G: -5312.08193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.71337 HOMO: -6.67767 LUMO: 2.34834 factor:1 | 1 (-1.26574) | -1 | -1 |
| G: -5312.08193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.48161 HOMO: -6.52801 LUMO: 2.10344 factor:1 | 1 (-1.03398) | -1 | -1 |
| G: -5312.08193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.53709 HOMO: -6.52801 LUMO: 2.24222 factor:1 | 1 (-1.08946) | -1 | -1 |
| G: -5312.08193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.56223 HOMO: -6.17154 LUMO: 1.89663 factor:1 | 1 (-1.11461) | -1 | -1 |
| G: -5312.08193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.74335 HOMO: -6.42733 LUMO: 2.15514 factor:1 | 1 (-1.29572) | -1 | -1 |
| G: -5312.08193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.69473 HOMO: -6.36474 LUMO: 2.01364 factor:1 | 1 (-1.24710) | -1 | -1 |
| G: -5312.08193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.60112 HOMO: -6.82189 LUMO: 1.86942 factor:1 | 1 (-1.15349) | -1 | -1 |
| G: -5312.08193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.88172 HOMO: -6.60148 LUMO: 2.00548 factor:1 | 1 (-1.43409) | -1 | -1 |
| G: -5312.08193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.58727 HOMO: -6.67767 LUMO: 2.15786 factor:1 | 1 (-1.13964) | -1 | -1 |
| G: -5312.08193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.75617 HOMO: -6.79196 LUMO: 2.06534 factor:1 | 1 (-1.30854) | -1 | -1 |
| G: -5312.08193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.61453 HOMO: -6.70216 LUMO: 1.83405 factor:1 | 1 (-1.16691) | -1 | -1 |
| G: -5312.08193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.53644 HOMO: -6.58788 LUMO: 1.79051 factor:1 | 1 (-1.08881) | -1 | -1 |
| G: -5312.08193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.42729 HOMO: -6.34842 LUMO: 1.80139 factor:1 | 1 (-0.97966) | -1 | -1 |
| G: -5312.08193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.44610 HOMO: -6.48175 LUMO: 1.95922 factor:1 | 1 (-0.99847) | -1 | -1 |
| G: -5312.08193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.71035 HOMO: -6.71033 LUMO: 2.02997 factor:1 | 1 (-1.26272) | -1 | -1 |
| G: -5312.08193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.81843 HOMO: -6.89264 LUMO: 2.42726 factor:1 | 1 (-1.37080) | -1 | -1 |
| G: -5312.08193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.60485 HOMO: -6.74570 LUMO: 2.20684 factor:1 | 1 (-1.15722) | -1 | -1 |
| G: -5312.08193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.39369 HOMO: -6.30216 LUMO: 2.15242 factor:1 | 1 (-0.94606) | -1 | -1 |
| G: -5312.08193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.43410 HOMO: -6.94979 LUMO: 2.43814 factor:1 | 1 (-0.98647) | -1 | -1 |
| G: -5312.08193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.32702 HOMO: -6.97972 LUMO: 2.11432 factor:1 | 1 (-0.87939) | -1 | -1 |
| G: -5312.08193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.18974 HOMO: -6.17154 LUMO: 1.98099 factor:1 | 1 (-0.74211) | -1 | -1 |
| G: -5312.08193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.70643 HOMO: -6.74026 LUMO: 2.21501 factor:1 | 1 (-1.25880) | -1 | -1 |
| G: -5312.08193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.48514 HOMO: -6.72393 LUMO: 2.19596 factor:1 | 1 (-1.03752) | -1 | -1 |
| G: -5312.08193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.14612 HOMO: -6.11440 LUMO: 2.10072 factor:1 | 1 (-0.69849) | -1 | -1 |
| G: -5312.08193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.21548 HOMO: -6.34297 LUMO: 1.92657 factor:1 | 1 (-0.76785) | -1 | -1 |
| G: -5312.08193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.52841 HOMO: -6.24773 LUMO: 2.00276 factor:1 | 1 (-1.08078) | -1 | -1 |
| G: -5312.08193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.30457 HOMO: -6.75114 LUMO: 1.98643 factor:1 | 1 (-0.85694) | -1 | -1 |
| G: -5312.08193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.37135 HOMO: -6.69128 LUMO: 2.08711 factor:1 | 1 (-0.92372) | -1 | -1 |
| G: -5312.08193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11578.10940 HOMO: -6.65318 LUMO: 2.15514 factor:1 | 1 (-1.66177) | -1 | -1 |
| G: -5312.08193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11578.39055 HOMO: -6.67495 LUMO: 1.72248 factor:1 | 1 (-1.94292) | -1 | -1 |
| G: -5312.08193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11578.98925 HOMO: -6.58243 LUMO: 1.83405 factor:1 | 1 (-2.54163) | -1 | -1 |
| G: -5312.08193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.70591 HOMO: -6.61237 LUMO: 1.69799 factor:1 | 1 (-1.25828) | -1 | -1 |
| G: -5312.08193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11578.13473 HOMO: -6.57427 LUMO: 2.29936 factor:1 | 1 (-1.68711) | -1 | -1 |
| G: -5312.08193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.74743 HOMO: -6.40012 LUMO: 2.35378 factor:1 | 1 (-1.29981) | -1 | -1 |
| G: -5312.08193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11578.17299 HOMO: -6.90081 LUMO: 2.26671 factor:1 | 1 (-1.72537) | -1 | -1 |
| G: -5312.08193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.99476 HOMO: -6.44910 LUMO: 2.25855 factor:1 | 1 (-1.54713) | -1 | -1 |
| G: -5312.08193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11578.38946 HOMO: -6.61509 LUMO: 2.26943 factor:1 | 1 (-1.94183) | -1 | -1 |
| G: -5312.08193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11578.93761 HOMO: -6.78924 LUMO: 2.09256 factor:1 | 1 (-2.48998) | -1 | -1 |
| G: -5312.08193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11578.19879 HOMO: -6.47087 LUMO: 1.97555 factor:1 | 1 (-1.75116) | -1 | -1 |
| G: -5312.08193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11578.45123 HOMO: -6.75931 LUMO: 1.98643 factor:1 | 1 (-2.00360) | -1 | -1 |
| G: -5312.08193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11579.10898 HOMO: -6.17971 LUMO: 2.09800 factor:1 | 1 (-2.66136) | -1 | -1 |
| G: -5312.08193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11578.98863 HOMO: -6.83006 LUMO: 1.91840 factor:1 | 1 (-2.54100) | -1 | -1 |
| G: -5312.08193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.81339 HOMO: -6.72938 LUMO: 2.17419 factor:1 | 1 (-1.36577) | -1 | -1 |
| G: -5312.08193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.96306 HOMO: -6.78924 LUMO: 2.42726 factor:1 | 1 (-1.51543) | -1 | -1 |
| G: -5312.08193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11578.29947 HOMO: -6.41372 LUMO: 1.93745 factor:1 | 1 (-1.85184) | -1 | -1 |
| G: -5312.08193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11578.18761 HOMO: -6.85455 LUMO: 2.14970 factor:1 | 1 (-1.73998) | -1 | -1 |
| G: -5312.08193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.91223 HOMO: -6.38651 LUMO: 2.18507 factor:1 | 1 (-1.46460) | -1 | -1 |
| G: -5312.08193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.69005 HOMO: -6.81373 LUMO: 2.00548 factor:1 | 1 (-0.24243) | -1 | -1 |
| G: -5312.08193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.85564 HOMO: -6.64774 LUMO: 2.41365 factor:1 | 1 (-0.40801) | -1 | -1 |
| G: -5312.08193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.10307 HOMO: -6.70489 LUMO: 2.31569 factor:1 | 1 (-0.65544) | -1 | -1 |
| G: -5312.08193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.79169 HOMO: -6.49264 LUMO: 1.78779 factor:1 | 1 (-0.34406) | -1 | -1 |
| G: -5312.08193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.60589 HOMO: -6.81101 LUMO: 1.86670 factor:1 | 1 (-0.15826) | -1 | -1 |
| G: -5312.08193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.64028 HOMO: -6.72121 LUMO: 1.48846 factor:1 | 1 (-0.19266) | -1 | -1 |
| G: -5312.08193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.65004 HOMO: -6.35930 LUMO: 1.78507 factor:1 | 1 (-1.20242) | -1 | -1 |
| G: -5312.08193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11578.51580 HOMO: -6.38651 LUMO: 2.04358 factor:1 | 1 (-2.06817) | -1 | -1 |
| G: -5312.08193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.97723 HOMO: -6.42189 LUMO: 1.99187 factor:1 | 1 (-1.52961) | -1 | -1 |
| G: -5312.08193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.83108 HOMO: -6.69400 LUMO: 1.61091 factor:1 | 1 (-1.38345) | -1 | -1 |
| G: -5312.08193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.58085 HOMO: -6.81101 LUMO: 2.17419 factor:1 | 1 (-1.13322) | -1 | -1 |
| G: -5312.08193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.70308 HOMO: -6.90897 LUMO: 2.28576 factor:1 | 1 (-1.25545) | -1 | -1 |
| G: -5312.08193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.59279 HOMO: -6.75387 LUMO: 2.31297 factor:1 | 1 (-1.14516) | -1 | -1 |
| G: -5312.08193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.80050 HOMO: -7.05863 LUMO: 2.18780 factor:1 | 1 (-1.35287) | -1 | -1 |
| G: -5312.08193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.65772 HOMO: -6.56611 LUMO: 1.99187 factor:1 | 1 (-1.21009) | -1 | -1 |
| G: -5312.08193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.96877 HOMO: -6.59060 LUMO: 1.86398 factor:1 | 1 (-1.52114) | -1 | -1 |
| G: -5312.08193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.76395 HOMO: -6.59060 LUMO: 1.59459 factor:1 | 1 (-1.31632) | -1 | -1 |
| G: -5312.08193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11578.12815 HOMO: -6.57699 LUMO: 1.48030 factor:1 | 1 (-1.68052) | -1 | -1 |
| G: -5312.08193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.97669 HOMO: -6.99605 LUMO: 2.30208 factor:1 | 1 (-1.52906) | -1 | -1 |
| G: -5312.08193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11578.22407 HOMO: -6.42189 LUMO: 2.20412 factor:1 | 1 (-1.77644) | -1 | -1 |
| G: -5312.08193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11578.80087 HOMO: -7.15115 LUMO: 1.83405 factor:1 | 1 (-2.35324) | 1 | 1 |
| G: -5312.08193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11578.38970 HOMO: -7.08040 LUMO: 2.21773 factor:1 | 1 (-1.94208) | 1 | 1 |
| G: -5312.08193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11578.15218 HOMO: -6.72121 LUMO: 1.89663 factor:1 | 1 (-1.70455) | -1 | -1 |
| G: -5312.08193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.71168 HOMO: -6.25590 LUMO: 1.85037 factor:1 | 1 (-1.26405) | -1 | -1 |
| G: -5312.08193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.95879 HOMO: -6.70489 LUMO: 1.98915 factor:1 | 1 (-1.51116) | -1 | -1 |
| G: -5312.08193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.95217 HOMO: -6.53617 LUMO: 2.08439 factor:1 | 1 (-1.50454) | -1 | -1 |
| G: -5312.08193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.82006 HOMO: -6.69944 LUMO: 1.98915 factor:1 | 1 (-1.37243) | -1 | -1 |
| G: -5312.08193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.56789 HOMO: -6.79468 LUMO: 1.96466 factor:1 | 1 (-1.12027) | -1 | -1 |
| G: -5312.08193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.91496 HOMO: -6.79468 LUMO: 1.99459 factor:1 | 1 (-0.46733) | -1 | -1 |
| G: -5312.08193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.82407 HOMO: -6.58788 LUMO: 1.98371 factor:1 | 1 (-0.37644) | -1 | -1 |
| G: -5312.08193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.93324 HOMO: -6.58788 LUMO: 2.16603 factor:1 | 1 (-0.48561) | -1 | -1 |
| G: -5312.08193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.17480 HOMO: -6.56883 LUMO: 1.64085 factor:1 | 1 (-0.72717) | -1 | -1 |
| G: -5312.08193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.12565 HOMO: -7.19197 LUMO: 2.66127 factor:1 | 1 (-0.67803) | 1 | 1 |
| G: -5312.08193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.96225 HOMO: -6.48175 LUMO: 2.40004 factor:1 | 1 (-0.51462) | -1 | -1 |
| G: -5312.08193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.93771 HOMO: -6.18515 LUMO: 2.27759 factor:1 | 1 (-0.49008) | -1 | -1 |
| G: -5312.08193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.74475 HOMO: -6.64774 LUMO: 2.13337 factor:1 | 1 (-0.29712) | -1 | -1 |
| G: -5312.08193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.76276 HOMO: -6.39740 LUMO: 1.95106 factor:1 | 1 (-0.31514) | -1 | -1 |
| G: -5312.08193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.68878 HOMO: -6.59332 LUMO: 1.81772 factor:1 | 1 (-0.24115) | -1 | -1 |
| G: -5312.08193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.82366 HOMO: -6.68312 LUMO: 2.41909 factor:1 | 1 (-0.37603) | -1 | -1 |
| G: -5312.08193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.95049 HOMO: -5.87494 LUMO: 2.18235 factor:1 | 1 (-0.50287) | -1 | -1 |
| G: -5312.08193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.92440 HOMO: -6.30488 LUMO: 2.04902 factor:1 | 1 (-0.47677) | -1 | -1 |
| G: -5312.08193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.05412 HOMO: -6.65046 LUMO: 2.05446 factor:1 | 1 (-0.60649) | -1 | -1 |
| G: -5312.08193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.09031 HOMO: -6.55794 LUMO: 2.06807 factor:1 | 1 (-0.64268) | -1 | -1 |
| G: -5312.08193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.87694 HOMO: -6.68040 LUMO: 1.99187 factor:1 | 1 (-0.42931) | -1 | -1 |
| G: -5312.08193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.82834 HOMO: -6.60965 LUMO: 2.18780 factor:1 | 1 (-0.38071) | -1 | -1 |
| G: -5312.08193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.66026 HOMO: -6.88176 LUMO: 2.10344 factor:1 | 1 (-0.21263) | -1 | -1 |
| G: -5312.08193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.80815 HOMO: -6.63414 LUMO: 1.70615 factor:1 | 1 (-0.36052) | -1 | -1 |
| G: -5312.08193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.68761 HOMO: -7.15115 LUMO: 2.07351 factor:1 | 1 (-0.23998) | 1 | 1 |
| G: -5312.08193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.85621 HOMO: -6.85727 LUMO: 2.27759 factor:1 | 1 (-0.40858) | -1 | -1 |
| G: -5312.08193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.69539 HOMO: -6.91713 LUMO: 2.28848 factor:1 | 1 (-0.24776) | -1 | -1 |
| G: -5312.08193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.11999 HOMO: -7.10217 LUMO: 2.14698 factor:1 | 1 (-0.67237) | 1 | 1 |
| G: -5312.08193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.89506 HOMO: -6.78108 LUMO: 2.45447 factor:1 | 1 (-0.44744) | -1 | -1 |
| G: -5312.08193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.90440 HOMO: -6.78380 LUMO: 2.43542 factor:1 | 1 (-0.45677) | -1 | -1 |
| G: -5312.08193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.75476 HOMO: -6.60965 LUMO: 2.33474 factor:1 | 1 (-0.30713) | -1 | -1 |
| G: -5312.08193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.67280 HOMO: -6.72665 LUMO: 2.25855 factor:1 | 1 (-0.22517) | -1 | -1 |
| G: -5312.08193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.55190 HOMO: -6.27495 LUMO: 2.04358 factor:1 | 1 (-0.10427) | -1 | -1 |
| G: -5312.08193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.70110 HOMO: -6.17426 LUMO: 1.45853 factor:1 | 1 (-0.25347) | -1 | -1 |
| G: -5312.08193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.94277 HOMO: -7.21374 LUMO: 2.33474 factor:1 | 1 (-0.49514) | 1 | 1 |
| G: -5312.08193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11578.14483 HOMO: -6.94707 LUMO: 1.81772 factor:1 | 1 (-1.69720) | -1 | -1 |
| G: -5312.08193 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11579.07984 HOMO: -6.80829 LUMO: 0.17960 factor:1 | 1 (-2.63221) | -1 | -1 |
| G: -5312.08193 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11578.29335 HOMO: -7.19469 LUMO: 1.60819 factor:1 | 1 (-1.84572) | 1 | 1 |
| G: -5312.08193 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11578.20937 HOMO: -6.78652 LUMO: 0.53334 factor:1 | 1 (-1.76175) | -1 | -1 |
| G: -5312.08193 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.98635 HOMO: -6.70489 LUMO: 0.74559 factor:1 | 1 (-1.53872) | -1 | -1 |
| G: -5312.08193 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.75493 HOMO: -6.72393 LUMO: 0.88981 factor:1 | 1 (-0.30730) | -1 | -1 |
| G: -5312.08193 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.73351 HOMO: -4.54430 LUMO: -0.90614 factor:1 | 1 (-0.28588) | -1 | -1 |
| G: -5312.08193 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.96571 HOMO: -6.83006 LUMO: 0.47348 factor:1 | 1 (-0.51808) | -1 | -1 |
| G: -5312.08193 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.84187 HOMO: -7.07496 LUMO: 0.50613 factor:1 | 1 (-0.39424) | -1 | -1 |
| G: -5312.08193 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.59903 HOMO: -6.62053 LUMO: 0.74559 factor:1 | 1 (-0.15140) | -1 | -1 |
| G: -5312.08193 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.50972 HOMO: -6.79196 LUMO: 1.80139 factor:1 | 1 (-0.06210) | -1 | -1 |
| G: -5312.08193 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.69416 HOMO: -6.71033 LUMO: 0.40817 factor:1 | 1 (-0.24654) | -1 | -1 |
| G: -5312.08193 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.87185 HOMO: -6.74026 LUMO: 0.95784 factor:1 | 1 (-0.42423) | -1 | -1 |
| G: -5312.08193 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.73758 HOMO: -7.34707 LUMO: 0.40001 factor:1 | 1 (-1.28996) | -1 | -1 |
| G: -5312.08193 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11578.44568 HOMO: -6.19875 LUMO: -0.88709 factor:1 | 1 (-1.99805) | -1 | -1 |
| G: -5312.08193 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.76953 HOMO: -6.48719 LUMO: -0.14694 factor:1 | 1 (-1.32190) | -1 | -1 |
| G: -5312.08193 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.97966 HOMO: -6.73482 LUMO: -0.01633 factor:1 | 1 (-1.53203) | -1 | -1 |
| G: -5312.08193 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.87266 HOMO: -7.05591 LUMO: -0.20136 factor:1 | 1 (-1.42503) | -1 | -1 |
| G: -5312.08193 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.59456 HOMO: -6.38651 LUMO: -2.07895 factor:1 | 1 (-1.14693) | -1 | -1 |
| G: -5312.08193 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.75707 HOMO: -6.85455 LUMO: -1.03403 factor:1 | 1 (-1.30944) | -1 | -1 |
| G: -5312.08193 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.92602 HOMO: -6.72121 LUMO: -0.99322 factor:1 | 1 (-1.47839) | -1 | -1 |
| G: -5312.08193 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.78575 HOMO: -6.53890 LUMO: -0.10885 factor:1 | 1 (-1.33812) | -1 | -1 |
| G: -5312.08193 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.54844 HOMO: -6.68312 LUMO: 0.21225 factor:1 | 1 (-1.10081) | -1 | -1 |
| G: -5312.08193 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11578.10545 HOMO: -6.68040 LUMO: 0.21225 factor:1 | 1 (-1.65783) | -1 | -1 |
| G: -5312.08193 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.93704 HOMO: -6.76475 LUMO: -0.64491 factor:1 | 1 (-1.48942) | -1 | -1 |
| G: -5312.08193 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11578.16984 HOMO: -6.48175 LUMO: 0.41633 factor:1 | 1 (-1.72221) | -1 | -1 |
| G: -5312.08193 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.91927 HOMO: -6.42733 LUMO: 0.16599 factor:1 | 1 (-1.47165) | -1 | -1 |
| G: -5312.08193 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11578.07949 HOMO: -6.66679 LUMO: 0.77825 factor:1 | 1 (-1.63187) | -1 | -1 |
| G: -5312.08193 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.76567 HOMO: -6.75931 LUMO: -0.73471 factor:1 | 1 (-0.31805) | -1 | -1 |
| G: -5312.08193 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.54853 HOMO: -6.53617 LUMO: 0.38096 factor:1 | 1 (-0.10090) | -1 | -1 |
| G: -5312.08193 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.85596 HOMO: -6.34297 LUMO: 0.35375 factor:1 | 1 (-0.40833) | -1 | -1 |
| G: -5312.08193 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.59808 HOMO: -7.11850 LUMO: -0.03265 factor:1 | 1 (-0.15045) | -1 | -1 |
| G: -5312.08193 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.81115 HOMO: -5.21914 LUMO: 1.29798 factor:1 | 1 (-0.36352) | -1 | -1 |
| G: -5312.08193 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.78461 HOMO: -7.09129 LUMO: -0.66668 factor:1 | 1 (-0.33699) | -1 | -1 |
| G: -5312.08193 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.56692 HOMO: -6.96884 LUMO: -0.31021 factor:1 | 1 (-0.11929) | -1 | -1 |
| G: -5312.08193 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.54436 HOMO: -6.51713 LUMO: -0.59865 factor:1 | 1 (-0.09674) | -1 | -1 |
| G: -5312.08193 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.34899 HOMO: -6.69400 LUMO: -0.07075 factor:1 | -1 (0.09864) | -1 | -1 |
| G: -5312.08193 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.72344 HOMO: -5.28173 LUMO: 1.17281 factor:1 | 1 (-0.27581) | -1 | -1 |
| G: -5312.08193 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.74235 HOMO: -6.54434 LUMO: 0.32109 factor:1 | 1 (-1.29472) | -1 | -1 |
| G: -5312.08193 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.55516 HOMO: -6.79740 LUMO: -0.24762 factor:1 | 1 (-1.10753) | -1 | -1 |
| G: -5312.08193 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11578.59292 HOMO: -6.91986 LUMO: -0.14694 factor:1 | 1 (-2.14529) | -1 | -1 |
| G: -5312.08193 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.58553 HOMO: -6.75114 LUMO: 0.18504 factor:1 | 1 (-1.13790) | -1 | -1 |
| G: -5312.08193 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.82621 HOMO: -6.74842 LUMO: 0.69389 factor:1 | 1 (-1.37858) | -1 | -1 |
| G: -5312.08193 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.78539 HOMO: -7.01782 LUMO: 0.56600 factor:1 | 1 (-1.33777) | -1 | -1 |
| G: -5312.08193 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.81100 HOMO: -6.47359 LUMO: -0.56600 factor:1 | 1 (-1.36337) | -1 | -1 |
| G: -5312.08193 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.61336 HOMO: -6.63686 LUMO: -0.55783 factor:1 | 1 (-1.16574) | -1 | -1 |
| G: -5312.08193 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.80537 HOMO: -4.13885 LUMO: -2.05446 factor:1 | 1 (-1.35774) | -1 | -1 |
| G: -5312.08193 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.02780 HOMO: -6.34570 LUMO: 0.19864 factor:1 | 1 (-0.58017) | -1 | -1 |
| G: -5312.08193 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.89789 HOMO: -6.47903 LUMO: 0.24762 factor:1 | 1 (-0.45027) | -1 | -1 |
| G: -5312.08193 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.94946 HOMO: -6.15249 LUMO: 0.32109 factor:1 | 1 (-0.50183) | -1 | -1 |
| G: -5312.08193 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.06759 HOMO: -6.84366 LUMO: 0.29116 factor:1 | 1 (-0.61996) | -1 | -1 |
| G: -5312.08193 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.90641 HOMO: -6.34297 LUMO: 0.19864 factor:1 | 1 (-0.45878) | -1 | -1 |
| G: -5312.08193 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.71041 HOMO: -6.51168 LUMO: 0.30749 factor:1 | 1 (-0.26278) | -1 | -1 |
| G: -5312.08193 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.81270 HOMO: -6.79468 LUMO: -0.16599 factor:1 | 1 (-0.36507) | -1 | -1 |
| G: -5312.08193 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.96054 HOMO: -7.24095 LUMO: 0.15238 factor:1 | 1 (-0.51291) | -1 | -1 |
| G: -5312.08193 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.21268 HOMO: -7.06952 LUMO: -0.34558 factor:1 | 1 (-0.76505) | -1 | -1 |
| G: -5312.08193 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.08187 HOMO: -6.88176 LUMO: 0.02177 factor:1 | 1 (-0.63424) | -1 | -1 |
| G: -5312.08193 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.20574 HOMO: -6.37291 LUMO: -0.69117 factor:1 | 1 (-0.75811) | -1 | -1 |
| G: -5312.08193 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.07199 HOMO: -6.83278 LUMO: -0.59049 factor:1 | 1 (-0.62437) | -1 | -1 |
| G: -5312.08193 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.04816 HOMO: -6.57155 LUMO: -0.33470 factor:1 | 1 (-0.60053) | -1 | -1 |
| G: -5312.08193 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.85226 HOMO: -6.89537 LUMO: -0.58504 factor:1 | 1 (-0.40463) | -1 | -1 |
| G: -5312.08193 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.98435 HOMO: -6.57155 LUMO: -0.34831 factor:1 | 1 (-0.53672) | -1 | -1 |
| G: -5312.08193 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.01730 HOMO: -6.64774 LUMO: -0.95784 factor:1 | 1 (-0.56967) | -1 | -1 |
| G: -5312.08193 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.18955 HOMO: -6.91713 LUMO: -0.69933 factor:1 | 1 (-0.74192) | -1 | -1 |
| G: -5312.08193 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.97814 HOMO: -6.80557 LUMO: -0.65035 factor:1 | 1 (-0.53051) | -1 | -1 |
| G: -5312.08193 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.21940 HOMO: -7.26544 LUMO: -0.79729 factor:1 | 1 (-0.77177) | -1 | -1 |
| G: -5312.08193 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.05120 HOMO: -6.69128 LUMO: -0.16871 factor:1 | 1 (-0.60358) | -1 | -1 |
| G: -5312.08193 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.80480 HOMO: -6.88448 LUMO: 0.13061 factor:1 | 1 (-0.35718) | -1 | -1 |
| G: -5312.08193 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.98315 HOMO: -6.50352 LUMO: 0.12245 factor:1 | 1 (-0.53552) | -1 | -1 |
| G: -5312.08193 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.86979 HOMO: -6.56067 LUMO: 0.17687 factor:1 | 1 (-0.42216) | -1 | -1 |
| G: -5312.08193 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.76970 HOMO: -6.70216 LUMO: 0.25034 factor:1 | 1 (-0.32207) | -1 | -1 |
| G: -5312.08193 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.98927 HOMO: -6.51713 LUMO: -0.78369 factor:1 | 1 (-0.54164) | -1 | -1 |
| G: -5312.08193 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.84516 HOMO: -6.50352 LUMO: 0.12245 factor:1 | 1 (-0.39753) | -1 | -1 |
| G: -5312.08193 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.12816 HOMO: -6.22052 LUMO: -0.83811 factor:1 | 1 (-0.68053) | -1 | -1 |
| G: -5312.08193 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.92805 HOMO: -6.51168 LUMO: -0.76464 factor:1 | 1 (-0.48042) | -1 | -1 |
| G: -5312.08193 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.12729 HOMO: -7.14571 LUMO: -0.80274 factor:1 | 1 (-0.67966) | -1 | -1 |
| G: -5312.08193 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.93028 HOMO: -6.66679 LUMO: -0.88709 factor:1 | 1 (-0.48265) | -1 | -1 |
| G: -5312.08193 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.77710 HOMO: -6.76203 LUMO: -1.43948 factor:1 | 1 (-0.32948) | -1 | -1 |
| G: -5312.08193 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.84151 HOMO: -6.57427 LUMO: -1.62996 factor:1 | 1 (-0.39388) | -1 | -1 |
| G: -5312.08193 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.59060 HOMO: -5.05043 LUMO: 1.24900 factor:1 | 1 (-0.14297) | -1 | -1 |
| G: -5312.08193 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.63027 HOMO: -6.53345 LUMO: 0.23130 factor:1 | 1 (-0.18264) | -1 | -1 |
| G: -5312.08193 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.60276 HOMO: -7.18381 LUMO: -0.22585 factor:1 | 1 (-0.15513) | -1 | -1 |
| G: -5312.08193 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.47770 HOMO: -7.00965 LUMO: -1.79595 factor:1 | 1 (-0.03007) | -1 | -1 |
| G: -5312.08193 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.97346 HOMO: -6.08174 LUMO: -0.82995 factor:1 | 1 (-0.52583) | -1 | -1 |
| G: -5312.08193 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.07588 HOMO: -6.42189 LUMO: -0.84355 factor:1 | 1 (-0.62826) | -1 | -1 |
| G: -5312.08193 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.02892 HOMO: -6.53890 LUMO: 0.60409 factor:1 | 1 (-0.58129) | -1 | -1 |
| G: -5312.08193 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.90965 HOMO: -6.62869 LUMO: 0.43810 factor:1 | 1 (-0.46202) | -1 | -1 |
| G: -5312.08193 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.13540 HOMO: -6.68312 LUMO: 0.64491 factor:1 | 1 (-0.68777) | -1 | -1 |
| G: -5312.08193 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.24680 HOMO: -6.42189 LUMO: 1.51295 factor:1 | 1 (-0.79917) | -1 | -1 |
| G: -5312.08193 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.13428 HOMO: -6.17971 LUMO: 1.67622 factor:1 | 1 (-0.68665) | -1 | -1 |
| G: -5312.08193 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.15844 HOMO: -6.79196 LUMO: 1.36873 factor:1 | 1 (-0.71082) | -1 | -1 |
| G: -5312.08193 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.02046 HOMO: -7.38517 LUMO: 0.56328 factor:1 | 1 (-0.57283) | 1 | 1 |
| G: -5312.08193 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.83944 HOMO: -7.56204 LUMO: 0.71566 factor:1 | 1 (-0.39182) | 1 | 1 |
| G: -5312.08193 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.77604 HOMO: -6.45726 LUMO: -1.91840 factor:1 | 1 (-0.32841) | -1 | -1 |
| G: -5312.08193 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.79210 HOMO: -6.13073 LUMO: -0.97417 factor:1 | 1 (-0.34447) | -1 | -1 |
| G: -5312.08193 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.98617 HOMO: -6.50352 LUMO: -0.69661 factor:1 | 1 (-0.53854) | -1 | -1 |
| G: -5312.08193 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.66085 HOMO: -6.76747 LUMO: -1.71976 factor:1 | 1 (-1.21322) | -1 | -1 |
| G: -5312.08193 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.42819 HOMO: -6.48447 LUMO: -0.89525 factor:1 | 1 (-0.98056) | -1 | -1 |
| G: -5312.08193 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.75987 HOMO: -7.11850 LUMO: -0.71566 factor:1 | 1 (-1.31224) | -1 | -1 |
| G: -5312.08193 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.91451 HOMO: -6.80285 LUMO: -0.49253 factor:1 | 1 (-1.46688) | -1 | -1 |
| G: -5312.08193 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.72196 HOMO: -6.80557 LUMO: -0.88165 factor:1 | 1 (-1.27434) | -1 | -1 |
| G: -5312.08193 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.96485 HOMO: -6.94162 LUMO: -0.08980 factor:1 | 1 (-1.51723) | -1 | -1 |
| G: -5312.08193 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.49037 HOMO: -6.97972 LUMO: -0.29388 factor:1 | 1 (-1.04274) | -1 | -1 |
| G: -5312.08193 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.46819 HOMO: -6.75114 LUMO: 0.04626 factor:1 | 1 (-1.02056) | -1 | -1 |
| G: -5312.08193 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.34155 HOMO: -7.15932 LUMO: 0.68845 factor:1 | 1 (-0.89392) | 1 | 1 |
| G: -5312.08193 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.64501 HOMO: -7.36612 LUMO: 0.63675 factor:1 | 1 (-1.19738) | 1 | 1 |
| G: -5312.08193 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.70632 HOMO: -7.02598 LUMO: -0.66124 factor:1 | 1 (-1.25869) | -1 | -1 |
| G: -5312.08193 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.79822 HOMO: -6.89264 LUMO: -0.54967 factor:1 | 1 (-0.35059) | -1 | -1 |
| G: -5312.08193 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.84396 HOMO: -6.97700 LUMO: 0.27756 factor:1 | 1 (-0.39633) | -1 | -1 |
| G: -5312.08193 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.08105 HOMO: -6.60965 LUMO: 0.08163 factor:1 | 1 (-0.63343) | -1 | -1 |
| G: -5312.08193 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.68439 HOMO: -6.70761 LUMO: 0.40001 factor:1 | 1 (-0.23677) | -1 | -1 |
| G: -5312.08193 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.87164 HOMO: -6.69128 LUMO: 0.23674 factor:1 | 1 (-0.42401) | -1 | -1 |
| G: -5312.08193 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.73591 HOMO: -6.69128 LUMO: -0.69933 factor:1 | 1 (-0.28828) | -1 | -1 |
| G: -5312.08193 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.89139 HOMO: -6.18515 LUMO: -0.85988 factor:1 | 1 (-0.44376) | -1 | -1 |
| G: -5312.08193 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.15583 HOMO: -6.86815 LUMO: -1.90208 factor:1 | 1 (-0.70820) | -1 | -1 |
| G: -5312.08193 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.85346 HOMO: -6.37563 LUMO: -1.74697 factor:1 | 1 (-0.40583) | -1 | -1 |
| G: -5312.08193 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.84862 HOMO: -6.75659 LUMO: 0.36463 factor:1 | 1 (-0.40099) | -1 | -1 |
| G: -5312.08193 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.71857 HOMO: -6.91441 LUMO: -0.88981 factor:1 | 1 (-0.27094) | -1 | -1 |
| G: -5312.08193 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.41503 HOMO: -6.71305 LUMO: -0.29933 factor:1 | -1 (0.03260) | -1 | -1 |
| G: -5312.08193 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.74089 HOMO: -6.91441 LUMO: -1.04492 factor:1 | 1 (-0.29326) | -1 | -1 |
| G: -5312.08193 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.96562 HOMO: -6.05453 LUMO: -0.83539 factor:1 | 1 (-0.51800) | -1 | -1 |
| G: -5312.08193 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.63555 HOMO: -7.35252 LUMO: -0.45715 factor:1 | 1 (-0.18792) | -1 | -1 |
| G: -5312.08193 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.75743 HOMO: -6.41644 LUMO: -0.97417 factor:1 | 1 (-0.30980) | -1 | -1 |
| G: -5312.08193 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.54842 HOMO: -6.78924 LUMO: 0.36735 factor:1 | 1 (-0.10079) | -1 | -1 |
| G: -5312.08193 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.11017 HOMO: -6.74298 LUMO: 0.51974 factor:1 | 1 (-0.66254) | -1 | -1 |
| G: -5312.08193 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.75640 HOMO: -6.48992 LUMO: 1.44765 factor:1 | 1 (-0.30877) | -1 | -1 |
| G: -5312.08193 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.62377 HOMO: -6.12528 LUMO: 1.57826 factor:1 | 1 (-0.17614) | -1 | -1 |
| G: -5312.08193 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.77509 HOMO: -6.62325 LUMO: 1.57826 factor:1 | 1 (-0.32746) | -1 | -1 |
| G: -5312.08193 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.97354 HOMO: -6.19875 LUMO: 1.29798 factor:1 | 1 (-0.52591) | -1 | -1 |
| G: -5312.08193 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.72023 HOMO: -6.74570 LUMO: 1.52112 factor:1 | 1 (-0.27260) | -1 | -1 |
| G: -5312.08193 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.50423 HOMO: -6.84094 LUMO: 1.48574 factor:1 | 1 (-0.05660) | -1 | -1 |
| G: -5312.08193 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.76668 HOMO: -6.85183 LUMO: 0.33470 factor:1 | 1 (-0.31905) | -1 | -1 |
| G: -5312.08193 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.78328 HOMO: -6.51168 LUMO: 0.48164 factor:1 | 1 (-0.33565) | -1 | -1 |
| G: -5312.08193 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.83596 HOMO: -6.25046 LUMO: 0.75648 factor:1 | 1 (-0.38833) | -1 | -1 |
| G: -5312.08193 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.87879 HOMO: -6.65591 LUMO: 0.32109 factor:1 | 1 (-0.43116) | -1 | -1 |
| G: -5312.08193 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.06726 HOMO: -6.71033 LUMO: 0.40817 factor:1 | 1 (-0.61963) | -1 | -1 |
| G: -5312.08193 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.90992 HOMO: -6.75114 LUMO: 0.73471 factor:1 | 1 (-0.46229) | -1 | -1 |
| G: -5312.08193 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.82649 HOMO: -6.50624 LUMO: 0.59321 factor:1 | 1 (-0.37886) | -1 | -1 |
| G: -5312.08193 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.70554 HOMO: -6.39740 LUMO: 0.83267 factor:1 | 1 (-0.25791) | -1 | -1 |
| G: -5312.08193 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.90200 HOMO: -6.44094 LUMO: 0.65579 factor:1 | 1 (-0.45438) | -1 | -1 |
| G: -5312.08193 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.74407 HOMO: -6.52257 LUMO: 0.05714 factor:1 | 1 (-0.29644) | -1 | -1 |
| G: -5312.08193 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.78516 HOMO: -7.10217 LUMO: 0.49797 factor:1 | 1 (-0.33753) | -1 | -1 |
| G: -5312.08193 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.54807 HOMO: -6.83006 LUMO: 0.55783 factor:1 | 1 (-0.10044) | -1 | -1 |
| G: -5312.08193 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.60782 HOMO: -6.99333 LUMO: -0.79457 factor:1 | 1 (-0.16019) | -1 | -1 |
| G: -5312.08193 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.43008 HOMO: -6.64230 LUMO: 0.32382 factor:1 | -1 (0.01755) | -1 | -1 |
| G: -5312.08193 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.74780 HOMO: -6.90897 LUMO: 0.30749 factor:1 | 1 (-0.30017) | -1 | -1 |
| G: -5312.08193 HOMO: -7.26544 LUMO: -1.10478 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.09861 HOMO: -7.09129 LUMO: 1.33336 factor:1 | 1 (-0.65098) | 1 | 1 |
| G: -5312.08193 HOMO: -7.26544 LUMO: -1.10478 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.96581 HOMO: -6.66951 LUMO: 1.34424 factor:1 | 1 (-0.51819) | -1 | -1 |
| G: -5312.08193 HOMO: -7.26544 LUMO: -1.10478 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.06669 HOMO: -7.02870 LUMO: 1.48574 factor:1 | 1 (-0.61906) | -1 | -1 |
| G: -5312.08193 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.95052 HOMO: -7.26544 LUMO: 0.32926 factor:1 | 1 (-0.50289) | -1 | -1 |
| G: -5312.08193 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.89381 HOMO: -6.56067 LUMO: -0.45987 factor:1 | 1 (-0.44619) | -1 | -1 |
| G: -5312.08193 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.75468 HOMO: -6.54434 LUMO: -0.28300 factor:1 | 1 (-0.30705) | -1 | -1 |
| G: -5312.08193 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.78323 HOMO: -7.19469 LUMO: 0.54695 factor:1 | 1 (-0.33560) | -1 | -1 |
| G: -5312.08193 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.71925 HOMO: -6.47359 LUMO: -0.22041 factor:1 | 1 (-0.27162) | -1 | -1 |
| G: -5312.08193 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.99975 HOMO: -6.80013 LUMO: 2.08167 factor:1 | 1 (-0.55212) | -1 | -1 |
| G: -5312.08193 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.68366 HOMO: -6.23957 LUMO: 1.67894 factor:1 | 1 (-0.23603) | -1 | -1 |
| G: -5312.08193 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.91482 HOMO: -6.75114 LUMO: -0.62858 factor:1 | 1 (-0.46719) | -1 | -1 |
| G: -5312.08193 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.63188 HOMO: -6.79468 LUMO: -0.64491 factor:1 | 1 (-0.18425) | -1 | -1 |
| G: -5312.08193 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.78793 HOMO: -6.84911 LUMO: -0.69661 factor:1 | 1 (-0.34031) | -1 | -1 |
| G: -5312.08193 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.48265 HOMO: -7.54028 LUMO: 0.25851 factor:1 | 1 (-0.03502) | -1 | -1 |
| G: -5312.08193 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.77427 HOMO: -6.92802 LUMO: -0.71022 factor:1 | 1 (-0.32665) | -1 | -1 |
| G: -5312.08193 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.60766 HOMO: -6.72665 LUMO: -0.46804 factor:1 | 1 (-0.16003) | -1 | -1 |
| G: -5312.08193 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.65694 HOMO: -6.63686 LUMO: -0.23674 factor:1 | 1 (-0.20931) | -1 | -1 |
| G: -5312.08193 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.39843 HOMO: -7.21102 LUMO: 0.54423 factor:1 | -1 (0.04920) | -1 | -1 |
| G: -5312.08193 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.97479 HOMO: -6.63414 LUMO: -0.25034 factor:1 | 1 (-0.52717) | -1 | -1 |
| G: -5312.08193 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.03743 HOMO: -6.70761 LUMO: -0.31837 factor:1 | 1 (-0.58981) | -1 | -1 |
| G: -5312.08193 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.13760 HOMO: -6.57155 LUMO: 1.76874 factor:1 | 1 (-0.68997) | -1 | -1 |
| G: -5312.08193 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.09050 HOMO: -6.84366 LUMO: 2.04358 factor:1 | 1 (-0.64287) | -1 | -1 |
| G: -5312.08193 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.11341 HOMO: -6.60420 LUMO: 1.80139 factor:1 | 1 (-0.66578) | -1 | -1 |
| G: -5312.08193 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.85264 HOMO: -7.03686 LUMO: 2.21229 factor:1 | 1 (-0.40501) | -1 | -1 |
| G: -5312.08193 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.86195 HOMO: -6.77564 LUMO: 1.97555 factor:1 | 1 (-0.41432) | -1 | -1 |
| G: -5312.08193 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.26843 HOMO: -6.40012 LUMO: 2.17691 factor:1 | 1 (-0.82080) | -1 | -1 |
| G: -5312.08193 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.09311 HOMO: -6.80013 LUMO: 2.25582 factor:1 | 1 (-0.64548) | -1 | -1 |
| G: -5312.08193 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.16642 HOMO: -6.74298 LUMO: 2.31569 factor:1 | 1 (-0.71879) | -1 | -1 |
| G: -5312.08193 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.03765 HOMO: -6.68856 LUMO: 1.85854 factor:1 | 1 (-0.59002) | -1 | -1 |
| G: -5312.08193 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.96701 HOMO: -6.17971 LUMO: 1.52928 factor:1 | 1 (-0.51938) | -1 | -1 |
| G: -5312.08193 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.95469 HOMO: -6.54162 LUMO: 1.91840 factor:1 | 1 (-0.50706) | -1 | -1 |
| G: -5312.08193 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.96048 HOMO: -6.80013 LUMO: -0.55511 factor:1 | 1 (-0.51285) | -1 | -1 |
| G: -5312.08193 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.07602 HOMO: -7.46953 LUMO: 0.28572 factor:1 | 1 (-0.62839) | -1 | -1 |
| G: -5312.08193 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.20103 HOMO: -6.61781 LUMO: -0.54967 factor:1 | 1 (-0.75340) | -1 | -1 |
| G: -5312.08193 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.24808 HOMO: -6.56339 LUMO: -0.47892 factor:1 | 1 (-0.80045) | -1 | -1 |
| G: -5312.08193 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.09031 HOMO: -6.65591 LUMO: -0.25307 factor:1 | 1 (-0.64268) | -1 | -1 |
| G: -5312.08193 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.04266 HOMO: -6.62869 LUMO: -0.23402 factor:1 | 1 (-0.59503) | -1 | -1 |
| G: -5312.08193 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.75539 HOMO: -6.58243 LUMO: -0.19048 factor:1 | 1 (-0.30776) | -1 | -1 |
| G: -5312.08193 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.75144 HOMO: -7.27632 LUMO: 0.52790 factor:1 | 1 (-0.30382) | -1 | -1 |
| G: -5312.08193 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.83623 HOMO: -7.21102 LUMO: 0.57688 factor:1 | 1 (-0.38861) | -1 | -1 |
| G: -5312.08193 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.10974 HOMO: -6.72393 LUMO: -0.53879 factor:1 | 1 (-0.66211) | -1 | -1 |
| G: -5312.08193 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.86965 HOMO: -7.42054 LUMO: -0.99322 factor:1 | 1 (-0.42202) | -1 | -1 |
| G: -5312.08193 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.16359 HOMO: -6.88992 LUMO: -0.71838 factor:1 | 1 (-0.71596) | -1 | -1 |
| G: -5312.08193 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.74208 HOMO: -6.88176 LUMO: -0.61226 factor:1 | 1 (-0.29445) | -1 | -1 |
| G: -5312.08193 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.93556 HOMO: -7.36340 LUMO: -1.04492 factor:1 | 1 (-0.48793) | -1 | -1 |
| G: -5312.08193 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.76067 HOMO: -6.65863 LUMO: -0.41906 factor:1 | 1 (-0.31304) | -1 | -1 |
| G: -5312.08193 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.54066 HOMO: -7.15115 LUMO: -0.66396 factor:1 | 1 (-0.09304) | -1 | -1 |
| G: -5312.08193 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.68371 HOMO: -7.10489 LUMO: -0.64491 factor:1 | 1 (-0.23609) | -1 | -1 |
| G: -5312.08193 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.86832 HOMO: -7.20285 LUMO: 0.47892 factor:1 | 1 (-0.42069) | -1 | -1 |
| G: -5312.08193 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.85022 HOMO: -6.55794 LUMO: -0.28844 factor:1 | 1 (-0.40259) | -1 | -1 |
| G: -5312.08193 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.12492 HOMO: -7.19197 LUMO: -0.69661 factor:1 | 1 (-0.67729) | -1 | -1 |
| G: -5312.08193 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.86192 HOMO: -6.56883 LUMO: -0.32926 factor:1 | 1 (-0.41429) | -1 | -1 |
| G: -5312.08193 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.96160 HOMO: -6.70761 LUMO: 1.95650 factor:1 | 1 (-0.51397) | -1 | -1 |
| G: -5312.08193 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.74148 HOMO: -6.60420 LUMO: 1.80684 factor:1 | 1 (-0.29386) | -1 | -1 |
| G: -5312.08193 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.05752 HOMO: -6.84094 LUMO: 1.64085 factor:1 | 1 (-0.60989) | -1 | -1 |
| G: -5312.08193 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.20187 HOMO: -6.69128 LUMO: 1.90208 factor:1 | 1 (-0.75425) | -1 | -1 |
| G: -5312.08193 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.82102 HOMO: -6.75387 LUMO: 1.70343 factor:1 | 1 (-0.37339) | -1 | -1 |
| G: -5312.08193 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.64412 HOMO: -7.07496 LUMO: 2.10072 factor:1 | 1 (-0.19649) | -1 | -1 |
| G: -5312.08193 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.94372 HOMO: -6.99877 LUMO: 2.24494 factor:1 | 1 (-0.49609) | -1 | -1 |
| G: -5312.08193 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.71166 HOMO: -6.63414 LUMO: 2.17691 factor:1 | 1 (-0.26403) | -1 | -1 |
| G: -5312.08193 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.63095 HOMO: -6.44638 LUMO: 1.78235 factor:1 | 1 (-0.18332) | -1 | -1 |
| G: -5312.08193 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.45688 HOMO: -6.87632 LUMO: 1.84221 factor:1 | 1 (-0.00925) | -1 | -1 |
| G: -5312.08193 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.96328 HOMO: -6.85183 LUMO: 1.68711 factor:1 | 1 (-0.51566) | -1 | -1 |
| G: -5312.08193 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.91428 HOMO: -6.96339 LUMO: 2.26671 factor:1 | 1 (-0.46665) | -1 | -1 |
| G: -5312.08193 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.16329 HOMO: -6.63141 LUMO: 1.96738 factor:1 | 1 (-0.71566) | -1 | -1 |
| G: -5312.08193 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.81452 HOMO: -6.37019 LUMO: 2.23133 factor:1 | 1 (-0.36689) | -1 | -1 |
| G: -5312.08193 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.68905 HOMO: -7.11034 LUMO: 2.32385 factor:1 | 1 (-0.24142) | 1 | 1 |
| G: -5312.08193 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.73563 HOMO: -6.91986 LUMO: 1.65445 factor:1 | 1 (-0.28801) | -1 | -1 |
| G: -5312.08193 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.96845 HOMO: -7.12938 LUMO: 2.28304 factor:1 | 1 (-0.52083) | 1 | 1 |
| G: -5312.08193 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.71142 HOMO: -6.54978 LUMO: 1.92112 factor:1 | 1 (-0.26379) | -1 | -1 |
| G: -5312.08193 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.72592 HOMO: -6.83006 LUMO: 2.48712 factor:1 | 1 (-0.27829) | -1 | -1 |
| G: -5312.08193 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.52129 HOMO: -6.97972 LUMO: 1.96738 factor:1 | 1 (-0.07366) | -1 | -1 |
| G: -5312.08193 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.59177 HOMO: -6.69944 LUMO: 2.06262 factor:1 | 1 (-0.14414) | -1 | -1 |
| G: -5312.08193 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.54140 HOMO: -6.76747 LUMO: 2.10888 factor:1 | 1 (-0.09377) | -1 | -1 |
| G: -5312.08193 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.32188 HOMO: -6.91169 LUMO: 2.06534 factor:1 | -1 (0.12574) | -1 | -1 |
| G: -5312.08193 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.75631 HOMO: -7.03414 LUMO: 1.93473 factor:1 | 1 (-0.30869) | -1 | -1 |
| G: -5312.08193 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.63870 HOMO: -7.03142 LUMO: 2.52250 factor:1 | 1 (-1.19107) | -1 | -1 |
| G: -5312.08193 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.80153 HOMO: -6.34025 LUMO: 2.61229 factor:1 | 1 (-1.35390) | -1 | -1 |
| G: -5312.08193 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.67432 HOMO: -6.98788 LUMO: 2.28304 factor:1 | 1 (-1.22669) | -1 | -1 |
| G: -5312.08193 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.73644 HOMO: -6.97700 LUMO: 2.53882 factor:1 | 1 (-1.28881) | -1 | -1 |
| G: -5312.08193 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.96877 HOMO: -6.58788 LUMO: 1.94289 factor:1 | 1 (-1.52114) | -1 | -1 |
| G: -5312.08193 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.95876 HOMO: -6.78652 LUMO: 2.13609 factor:1 | 1 (-1.51113) | -1 | -1 |
| G: -5312.08193 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.90872 HOMO: -6.55250 LUMO: 1.82861 factor:1 | 1 (-1.46109) | -1 | -1 |
| G: -5312.08193 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.92774 HOMO: -6.45998 LUMO: 1.75786 factor:1 | 1 (-1.48011) | -1 | -1 |
| G: -5312.08193 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.65769 HOMO: -6.78924 LUMO: 2.33746 factor:1 | 1 (-1.21006) | -1 | -1 |
| G: -5312.08193 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.63043 HOMO: -6.85727 LUMO: 1.76058 factor:1 | 1 (-1.18280) | -1 | -1 |
| G: -5312.08193 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.45026 HOMO: -6.70489 LUMO: 1.84493 factor:1 | 1 (-1.00263) | -1 | -1 |
| G: -5312.08193 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.56498 HOMO: -6.71305 LUMO: 1.53472 factor:1 | 1 (-1.11735) | -1 | -1 |
| G: -5312.08193 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.49097 HOMO: -6.76747 LUMO: 1.48846 factor:1 | 1 (-1.04334) | -1 | -1 |
| G: -5312.08193 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.48065 HOMO: -6.69128 LUMO: 1.95922 factor:1 | 1 (-1.03303) | -1 | -1 |
| G: -5312.08193 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.65290 HOMO: -6.67495 LUMO: 2.05446 factor:1 | 1 (-1.20527) | -1 | -1 |
| G: -5312.08193 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.98152 HOMO: -6.63686 LUMO: 2.25310 factor:1 | 1 (-0.53389) | -1 | -1 |
| G: -5312.08193 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.05708 HOMO: -6.63958 LUMO: 2.14154 factor:1 | 1 (-0.60945) | -1 | -1 |
| G: -5312.08193 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.11439 HOMO: -6.62597 LUMO: 2.01908 factor:1 | 1 (-0.66676) | -1 | -1 |
| G: -5312.08193 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.17559 HOMO: -7.07768 LUMO: 2.14154 factor:1 | 1 (-0.72796) | -1 | -1 |
| G: -5312.08193 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.18280 HOMO: -6.19603 LUMO: 2.01092 factor:1 | 1 (-0.73517) | -1 | -1 |
| G: -5312.08193 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.11270 HOMO: -6.65046 LUMO: 2.15786 factor:1 | 1 (-0.66507) | -1 | -1 |
| G: -5312.08193 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.90410 HOMO: -6.92258 LUMO: 2.31841 factor:1 | 1 (-0.45647) | -1 | -1 |
| G: -5312.08193 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.87038 HOMO: -6.90081 LUMO: 2.19324 factor:1 | 1 (-0.42276) | -1 | -1 |
| G: -5312.08193 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.75283 HOMO: -6.85455 LUMO: 1.95650 factor:1 | 1 (-0.30520) | -1 | -1 |
| G: -5312.08193 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.90707 HOMO: -6.57699 LUMO: 1.76058 factor:1 | 1 (-0.45944) | -1 | -1 |
| G: -5312.08193 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.67103 HOMO: -6.90625 LUMO: 1.97555 factor:1 | 1 (-0.22341) | -1 | -1 |
| G: -5312.08193 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.89659 HOMO: -6.97428 LUMO: 1.92929 factor:1 | 1 (-0.44896) | -1 | -1 |
| G: -5312.08193 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.69893 HOMO: -6.61781 LUMO: -0.41906 factor:1 | 1 (-0.25130) | -1 | -1 |
| G: -5312.08193 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.93077 HOMO: -6.62869 LUMO: -0.81906 factor:1 | 1 (-0.48314) | -1 | -1 |
| G: -5312.08193 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.89904 HOMO: -7.01237 LUMO: 2.00548 factor:1 | 1 (-0.45141) | -1 | -1 |
| G: -5312.08193 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.77642 HOMO: -6.85727 LUMO: 2.17691 factor:1 | 1 (-0.32880) | -1 | -1 |
| G: -5312.08193 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.86100 HOMO: -6.71849 LUMO: 1.58914 factor:1 | 1 (-0.41337) | -1 | -1 |
| G: -5312.08193 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.59930 HOMO: -7.52395 LUMO: 0.27211 factor:1 | 1 (-0.15168) | -1 | -1 |
| G: -5312.08193 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.92663 HOMO: -6.96611 LUMO: -0.72654 factor:1 | 1 (-0.47900) | -1 | -1 |
| G: -5312.08193 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.68611 HOMO: -6.89537 LUMO: -0.68028 factor:1 | 1 (-0.23848) | -1 | -1 |
| G: -5312.08193 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.55683 HOMO: -6.84911 LUMO: -0.58504 factor:1 | 1 (-0.10920) | -1 | -1 |
| G: -5312.08193 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.51397 HOMO: -6.79196 LUMO: -0.55783 factor:1 | 1 (-0.06634) | -1 | -1 |
| G: -5312.08193 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.76355 HOMO: -6.67767 LUMO: 1.79323 factor:1 | 1 (-0.31592) | -1 | -1 |
| G: -5312.08193 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.57638 HOMO: -6.54434 LUMO: 1.91024 factor:1 | 1 (-1.12876) | -1 | -1 |
| G: -5312.08193 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.40958 HOMO: -6.62869 LUMO: 1.69799 factor:1 | 1 (-0.96195) | -1 | -1 |
| G: -5312.08193 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.54188 HOMO: -6.72393 LUMO: 2.12249 factor:1 | 1 (-1.09425) | -1 | -1 |
| G: -5312.08193 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.58384 HOMO: -6.66407 LUMO: 2.05990 factor:1 | 1 (-1.13621) | -1 | -1 |
| G: -5312.08193 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.70945 HOMO: -7.00149 LUMO: 1.82044 factor:1 | 1 (-1.26182) | -1 | -1 |
| G: -5312.08193 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.77786 HOMO: -7.12122 LUMO: 2.16058 factor:1 | 1 (-1.33023) | 1 | 1 |
| G: -5312.08193 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.55861 HOMO: -6.63141 LUMO: 2.21229 factor:1 | 1 (-1.11099) | -1 | -1 |
| G: -5312.08193 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.61418 HOMO: -6.37835 LUMO: 2.32113 factor:1 | 1 (-1.16655) | -1 | -1 |
| G: -5312.08193 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.50438 HOMO: -6.99605 LUMO: 2.00548 factor:1 | 1 (-1.05675) | -1 | -1 |
| G: -5312.08193 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.91176 HOMO: -6.85999 LUMO: 2.39460 factor:1 | 1 (-1.46414) | -1 | -1 |
| G: -5312.08193 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.48765 HOMO: -6.85727 LUMO: 2.48712 factor:1 | 1 (-1.04002) | -1 | -1 |
| G: -5312.08193 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.36862 HOMO: -7.04231 LUMO: 2.40277 factor:1 | 1 (-0.92100) | -1 | -1 |
| G: -5312.08193 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.25153 HOMO: -6.60692 LUMO: 2.26671 factor:1 | 1 (-0.80391) | -1 | -1 |
| G: -5312.08193 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.34509 HOMO: -6.67495 LUMO: 2.14698 factor:1 | 1 (-0.89746) | -1 | -1 |
| G: -5312.08193 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.64632 HOMO: -6.73210 LUMO: 2.06807 factor:1 | 1 (-1.19869) | -1 | -1 |
| G: -5312.08193 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.79182 HOMO: -7.20013 LUMO: 2.02181 factor:1 | 1 (-1.34419) | 1 | 1 |
| G: -5312.08193 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.57162 HOMO: -7.18653 LUMO: 2.29936 factor:1 | 1 (-1.12399) | 1 | 1 |
| G: -5312.08193 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.62871 HOMO: -6.92802 LUMO: 2.36195 factor:1 | 1 (-1.18108) | -1 | -1 |
| G: -5312.08193 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.87715 HOMO: -6.89537 LUMO: 1.78779 factor:1 | 1 (-1.42952) | -1 | -1 |
| G: -5312.08193 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.87813 HOMO: -6.96067 LUMO: 2.31297 factor:1 | 1 (-1.43050) | -1 | -1 |
| G: -5312.08193 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.57652 HOMO: -6.91441 LUMO: 2.50345 factor:1 | 1 (-1.12889) | -1 | -1 |
| G: -5312.08193 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.59940 HOMO: -7.17292 LUMO: 2.12521 factor:1 | 1 (-1.15178) | 1 | 1 |
| G: -5312.08193 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.48025 HOMO: -6.93618 LUMO: 2.35106 factor:1 | 1 (-1.03262) | -1 | -1 |
| G: -5312.08193 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.39891 HOMO: -6.75931 LUMO: 1.61908 factor:1 | 1 (-0.95128) | -1 | -1 |
| G: -5312.08193 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.41015 HOMO: -6.35930 LUMO: 1.23540 factor:1 | 1 (-0.96252) | -1 | -1 |
| G: -5312.08193 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.72392 HOMO: -6.17971 LUMO: 1.84493 factor:1 | 1 (-1.27630) | -1 | -1 |
| G: -5312.08193 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.55203 HOMO: -6.72665 LUMO: 2.61229 factor:1 | 1 (-1.10440) | -1 | -1 |
| G: -5312.08193 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.55497 HOMO: -6.62869 LUMO: 2.28304 factor:1 | 1 (-1.10734) | -1 | -1 |
| G: -5312.08193 HOMO: -8.88180 LUMO: 1.02315 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11578.15727 HOMO: -6.58243 LUMO: 0.28028 factor:1 | 1 (-1.70964) | -1 | -1 |
| G: -5312.08193 HOMO: -8.88180 LUMO: 1.02315 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11578.38769 HOMO: -6.79468 LUMO: 0.14966 factor:1 | 1 (-1.94006) | -1 | -1 |
| G: -5312.08193 HOMO: -8.88180 LUMO: 1.02315 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11578.98297 HOMO: -6.63141 LUMO: 0.31021 factor:1 | 1 (-2.53534) | -1 | -1 |
| G: -5312.08193 HOMO: -8.88180 LUMO: 1.02315 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.97255 HOMO: -6.81101 LUMO: 0.13878 factor:1 | 1 (-1.52493) | -1 | -1 |
| G: -5312.08193 HOMO: -8.88180 LUMO: 1.02315 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.96265 HOMO: -6.72665 LUMO: 0.65579 factor:1 | 1 (-1.51502) | -1 | -1 |
| G: -5312.08193 HOMO: -8.88180 LUMO: 1.02315 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11578.18861 HOMO: -6.53073 LUMO: 0.91430 factor:1 | 1 (-1.74098) | -1 | -1 |
| G: -5312.08193 HOMO: -8.88180 LUMO: 1.02315 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.99873 HOMO: -7.19197 LUMO: 1.62996 factor:1 | 1 (-1.55110) | 1 | 1 |
| G: -5312.08193 HOMO: -8.88180 LUMO: 1.02315 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.96820 HOMO: -6.69400 LUMO: 0.84627 factor:1 | 1 (-1.52057) | -1 | -1 |
| G: -5312.08193 HOMO: -8.88180 LUMO: 1.02315 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11578.19425 HOMO: -6.76475 LUMO: 0.51974 factor:1 | 1 (-1.74662) | -1 | -1 |
| G: -5312.08193 HOMO: -8.88180 LUMO: 1.02315 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.83141 HOMO: -6.67767 LUMO: 0.52246 factor:1 | 1 (-1.38378) | -1 | -1 |
| G: -5312.08193 HOMO: -8.88180 LUMO: 1.02315 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11578.98033 HOMO: -6.73210 LUMO: 0.94424 factor:1 | 1 (-2.53270) | -1 | -1 |
| G: -5312.08193 HOMO: -8.88180 LUMO: 1.02315 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11578.98218 HOMO: -6.97972 LUMO: 0.60409 factor:1 | 1 (-2.53455) | -1 | -1 |
| G: -5312.08193 HOMO: -8.88180 LUMO: 1.02315 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.79497 HOMO: -7.38517 LUMO: 0.73743 factor:1 | 1 (-1.34734) | -1 | -1 |
| G: -5312.08193 HOMO: -8.88180 LUMO: 1.02315 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11578.00496 HOMO: -6.48992 LUMO: 1.08301 factor:1 | 1 (-1.55733) | -1 | -1 |
| G: -5312.08193 HOMO: -8.88180 LUMO: 1.02315 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.93108 HOMO: -7.18381 LUMO: 1.61908 factor:1 | 1 (-1.48346) | 1 | 1 |
| G: -5312.08193 HOMO: -8.88180 LUMO: 1.02315 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.82882 HOMO: -6.74842 LUMO: 0.57960 factor:1 | 1 (-1.38120) | -1 | -1 |
| G: -5312.08193 HOMO: -8.88180 LUMO: 1.02315 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.58974 HOMO: -6.67495 LUMO: 0.77280 factor:1 | 1 (-1.14212) | -1 | -1 |
| G: -5312.08193 HOMO: -8.88180 LUMO: 1.02315 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11578.11101 HOMO: -6.74570 LUMO: 0.77280 factor:1 | 1 (-1.66338) | -1 | -1 |
| G: -5312.08193 HOMO: -8.88180 LUMO: 1.02315 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11578.38206 HOMO: -6.73754 LUMO: 0.86804 factor:1 | 1 (-1.93443) | -1 | -1 |
| G: -5312.08193 HOMO: -8.88180 LUMO: 1.02315 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11578.12611 HOMO: -6.66135 LUMO: 0.94424 factor:1 | 1 (-1.67848) | -1 | -1 |
| G: -5312.08193 HOMO: -8.88180 LUMO: 1.02315 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11578.10246 HOMO: -6.44638 LUMO: 1.00138 factor:1 | 1 (-1.65483) | -1 | -1 |
| G: -5312.08193 HOMO: -8.88180 LUMO: 1.02315 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.89930 HOMO: -6.65591 LUMO: 1.02043 factor:1 | 1 (-1.45167) | -1 | -1 |
| G: -5312.08193 HOMO: -8.88180 LUMO: 1.02315 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.80412 HOMO: -7.17564 LUMO: 0.50069 factor:1 | 1 (-0.35650) | -1 | -1 |
| G: -5312.08193 HOMO: -8.88180 LUMO: 1.02315 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.83515 HOMO: -6.59332 LUMO: 0.79457 factor:1 | 1 (-0.38752) | -1 | -1 |
| G: -5312.08193 HOMO: -8.88180 LUMO: 1.02315 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.02075 HOMO: -6.76747 LUMO: 1.73881 factor:1 | 1 (-0.57313) | -1 | -1 |
| G: -5312.08193 HOMO: -8.88180 LUMO: 1.02315 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.78886 HOMO: -7.00421 LUMO: 1.07485 factor:1 | 1 (-0.34123) | -1 | -1 |
| G: -5312.08193 HOMO: -8.88180 LUMO: 1.02315 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.73950 HOMO: -6.94979 LUMO: 1.67894 factor:1 | 1 (-0.29187) | -1 | -1 |
| G: -5312.08193 HOMO: -8.88180 LUMO: 1.02315 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.80244 HOMO: -6.66135 LUMO: 0.47076 factor:1 | 1 (-0.35481) | -1 | -1 |
| G: -5312.08193 HOMO: -8.88180 LUMO: 1.02315 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.59253 HOMO: -6.74298 LUMO: 1.85037 factor:1 | 1 (-0.14490) | -1 | -1 |
| G: -5312.08193 HOMO: -8.88180 LUMO: 1.02315 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.69710 HOMO: -6.65318 LUMO: 0.95240 factor:1 | 1 (-0.24947) | -1 | -1 |
| G: -5312.08193 HOMO: -8.88180 LUMO: 1.02315 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.88628 HOMO: -6.63958 LUMO: 0.78097 factor:1 | 1 (-0.43865) | -1 | -1 |
| G: -5312.08193 HOMO: -8.88180 LUMO: 1.02315 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.77851 HOMO: -6.11712 LUMO: 0.40001 factor:1 | 1 (-1.33088) | -1 | -1 |
| G: -5312.08193 HOMO: -8.88180 LUMO: 1.02315 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11578.60606 HOMO: -7.08312 LUMO: 0.92519 factor:1 | 1 (-2.15843) | -1 | -1 |
| G: -5312.08193 HOMO: -8.88180 LUMO: 1.02315 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.94219 HOMO: -6.96067 LUMO: 0.54695 factor:1 | 1 (-1.49456) | -1 | -1 |
| G: -5312.08193 HOMO: -8.88180 LUMO: 1.02315 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.83549 HOMO: -6.74026 LUMO: 0.60137 factor:1 | 1 (-1.38786) | -1 | -1 |
| G: -5312.08193 HOMO: -8.88180 LUMO: 1.02315 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.77712 HOMO: -6.74298 LUMO: 0.59593 factor:1 | 1 (-1.32949) | -1 | -1 |
| G: -5312.08193 HOMO: -8.88180 LUMO: 1.02315 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.57110 HOMO: -6.93074 LUMO: 0.60681 factor:1 | 1 (-1.12348) | -1 | -1 |
| G: -5312.08193 HOMO: -8.88180 LUMO: 1.02315 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.80442 HOMO: -6.41644 LUMO: 0.35919 factor:1 | 1 (-1.35679) | -1 | -1 |
| G: -5312.08193 HOMO: -8.88180 LUMO: 1.02315 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.61530 HOMO: -6.41917 LUMO: 1.73064 factor:1 | 1 (-1.16767) | -1 | -1 |
| G: -5312.08193 HOMO: -8.88180 LUMO: 1.02315 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.80771 HOMO: -4.64226 LUMO: -0.87893 factor:1 | 1 (-1.36008) | -1 | -1 |
| G: -5312.08193 HOMO: -8.88180 LUMO: 1.02315 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.65108 HOMO: -6.59604 LUMO: 0.90342 factor:1 | 1 (-1.20345) | -1 | -1 |
| G: -5312.08193 HOMO: -8.88180 LUMO: 1.02315 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.80096 HOMO: -6.79468 LUMO: 0.50069 factor:1 | 1 (-1.35333) | -1 | -1 |
| G: -5312.08193 HOMO: -8.88180 LUMO: 1.02315 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.76194 HOMO: -7.04503 LUMO: 0.52518 factor:1 | 1 (-1.31431) | -1 | -1 |
| G: -5312.08193 HOMO: -8.88180 LUMO: 1.02315 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.88070 HOMO: -6.69400 LUMO: 0.54423 factor:1 | 1 (-0.43307) | -1 | -1 |
| G: -5312.08193 HOMO: -8.88180 LUMO: 1.02315 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.90424 HOMO: -6.51713 LUMO: 0.95240 factor:1 | 1 (-0.45661) | -1 | -1 |
| G: -5312.08193 HOMO: -8.88180 LUMO: 1.02315 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.00598 HOMO: -6.88176 LUMO: 1.79323 factor:1 | 1 (-0.55835) | -1 | -1 |
| G: -5312.08193 HOMO: -8.88180 LUMO: 1.02315 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.12816 HOMO: -6.71849 LUMO: 0.28844 factor:1 | 1 (-0.68053) | -1 | -1 |
| G: -5312.08193 HOMO: -8.88180 LUMO: 1.02315 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.02026 HOMO: -6.94979 LUMO: 0.51974 factor:1 | 1 (-0.57264) | -1 | -1 |
| G: -5312.08193 HOMO: -8.88180 LUMO: 1.02315 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.92772 HOMO: -6.76203 LUMO: 0.94151 factor:1 | 1 (-0.48009) | -1 | -1 |
| G: -5312.08193 HOMO: -8.88180 LUMO: 1.02315 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.90870 HOMO: -6.91169 LUMO: 0.89525 factor:1 | 1 (-0.46107) | -1 | -1 |
| G: -5312.08193 HOMO: -8.88180 LUMO: 1.02315 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.04040 HOMO: -6.83006 LUMO: 0.89253 factor:1 | 1 (-0.59277) | -1 | -1 |
| G: -5312.08193 HOMO: -8.88180 LUMO: 1.02315 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.96747 HOMO: -7.08857 LUMO: 0.60409 factor:1 | 1 (-0.51985) | -1 | -1 |
| G: -5312.08193 HOMO: -8.88180 LUMO: 1.02315 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.68956 HOMO: -6.91713 LUMO: 1.76330 factor:1 | 1 (-0.24194) | -1 | -1 |
| G: -5312.08193 HOMO: -8.88180 LUMO: 1.02315 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.93128 HOMO: -6.47359 LUMO: 1.56193 factor:1 | 1 (-0.48366) | -1 | -1 |
| G: -5312.08193 HOMO: -6.91169 LUMO: -0.53879 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.76001 HOMO: -7.00149 LUMO: 1.47214 factor:1 | 1 (-0.31239) | -1 | -1 |
| G: -5312.08193 HOMO: -6.91169 LUMO: -0.53879 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.96421 HOMO: -7.03686 LUMO: 1.97283 factor:1 | 1 (-0.51658) | -1 | -1 |
| G: -5312.08193 HOMO: -6.91169 LUMO: -0.53879 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.01020 HOMO: -7.00965 LUMO: 1.64629 factor:1 | 1 (-0.56257) | -1 | -1 |
| G: -5312.08193 HOMO: -6.91169 LUMO: -0.53879 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.77836 HOMO: -7.06952 LUMO: 1.67622 factor:1 | 1 (-0.33073) | 1 | -1 |
| G: -5312.08193 HOMO: -6.91169 LUMO: -0.53879 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.00339 HOMO: -6.80557 LUMO: 1.70615 factor:1 | 1 (-0.55577) | -1 | -1 |
| G: -5312.08193 HOMO: -6.91169 LUMO: -0.53879 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.81721 HOMO: -6.80829 LUMO: 1.71704 factor:1 | 1 (-0.36959) | -1 | -1 |
| G: -5312.08193 HOMO: -6.91169 LUMO: -0.53879 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.98712 HOMO: -7.26544 LUMO: 1.89935 factor:1 | 1 (-0.53949) | 1 | -1 |
| G: -5312.08193 HOMO: -7.29809 LUMO: 2.83543 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.77871 HOMO: -7.00149 LUMO: 1.47214 factor:1 | 1 (-0.33108) | -1 | -1 |
| G: -5312.08193 HOMO: -7.29809 LUMO: 2.83543 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.09684 HOMO: -7.03686 LUMO: 1.97283 factor:1 | 1 (-0.64921) | -1 | -1 |
| G: -5312.08193 HOMO: -7.29809 LUMO: 2.83543 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.80837 HOMO: -7.00965 LUMO: 1.64629 factor:1 | 1 (-0.36074) | -1 | -1 |
| G: -5312.08193 HOMO: -7.29809 LUMO: 2.83543 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.56178 HOMO: -7.06952 LUMO: 1.67622 factor:1 | 1 (-0.11415) | -1 | -1 |
| G: -5312.08193 HOMO: -7.29809 LUMO: 2.83543 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.81928 HOMO: -6.80557 LUMO: 1.70615 factor:1 | 1 (-0.37165) | -1 | -1 |
| G: -5312.08193 HOMO: -7.29809 LUMO: 2.83543 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.04212 HOMO: -6.80829 LUMO: 1.71704 factor:1 | 1 (-0.59449) | -1 | -1 |
| G: -5312.08193 HOMO: -7.29809 LUMO: 2.83543 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.84208 HOMO: -7.26544 LUMO: 1.89935 factor:1 | 1 (-0.39446) | -1 | -1 |
| G: -5312.08193 HOMO: -7.85865 LUMO: 2.83543 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.93322 HOMO: -7.00149 LUMO: 1.75241 factor:1 | 1 (-0.48559) | -1 | -1 |
| G: -5312.08193 HOMO: -7.85865 LUMO: 2.83543 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.72227 HOMO: -6.91169 LUMO: 2.07079 factor:1 | 1 (-0.27464) | -1 | -1 |
| G: -5312.08193 HOMO: -7.85865 LUMO: 2.83543 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.04337 HOMO: -7.11034 LUMO: 1.76330 factor:1 | 1 (-0.59574) | -1 | -1 |
| G: -5312.08193 HOMO: -7.85865 LUMO: 2.83543 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.83278 HOMO: -6.87360 LUMO: 2.02725 factor:1 | 1 (-0.38515) | -1 | -1 |
| G: -5312.08193 HOMO: -7.85865 LUMO: 2.83543 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.79207 HOMO: -7.08584 LUMO: 1.82044 factor:1 | 1 (-0.34444) | -1 | -1 |
| G: -5312.08193 HOMO: -7.85865 LUMO: 2.83543 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.51941 HOMO: -6.90625 LUMO: 1.68166 factor:1 | 1 (-0.07178) | -1 | -1 |
| G: -5312.08193 HOMO: -7.85865 LUMO: 2.83543 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.88617 HOMO: -6.71577 LUMO: 1.93201 factor:1 | 1 (-0.43854) | -1 | -1 |
| G: -5312.08193 HOMO: -7.85865 LUMO: 2.83543 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.62926 HOMO: -6.99605 LUMO: 2.08439 factor:1 | 1 (-0.18164) | -1 | -1 |
| G: -5312.08193 HOMO: -7.85865 LUMO: 2.83543 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.44537 HOMO: -7.02326 LUMO: 1.97010 factor:1 | -1 (0.00226) | -1 | -1 |
| G: -5312.08193 HOMO: -7.85865 LUMO: 2.83543 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.64423 HOMO: -6.99877 LUMO: 2.15514 factor:1 | 1 (-0.19660) | -1 | -1 |
| G: -5312.08193 HOMO: -7.85865 LUMO: 2.83543 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.80597 HOMO: -6.75387 LUMO: 1.95106 factor:1 | 1 (-0.35835) | -1 | -1 |
| G: -5312.08193 HOMO: -7.85865 LUMO: 2.83543 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.78347 HOMO: -7.10761 LUMO: 2.06262 factor:1 | 1 (-0.33584) | -1 | -1 |
| G: -5312.08193 HOMO: -7.85865 LUMO: 2.83543 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.83830 HOMO: -7.03142 LUMO: 1.91568 factor:1 | 1 (-0.39067) | -1 | -1 |
| G: -5312.08193 HOMO: -7.85865 LUMO: 2.83543 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.88540 HOMO: -6.98788 LUMO: 1.98371 factor:1 | 1 (-0.43778) | -1 | -1 |
| G: -5312.08193 HOMO: -7.85865 LUMO: 2.83543 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.79493 HOMO: -6.94707 LUMO: 1.68438 factor:1 | 1 (-0.34730) | -1 | -1 |
| G: -5312.08193 HOMO: -7.85865 LUMO: 2.83543 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.75939 HOMO: -6.88176 LUMO: 2.20684 factor:1 | 1 (-0.31176) | -1 | -1 |
| G: -5312.08193 HOMO: -7.85865 LUMO: 2.83543 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.79498 HOMO: -6.73210 LUMO: 2.18780 factor:1 | 1 (-0.34735) | -1 | -1 |
| G: -5312.08193 HOMO: -7.85865 LUMO: 2.83543 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.94500 HOMO: -6.83822 LUMO: 2.06807 factor:1 | 1 (-0.49737) | -1 | -1 |
| G: -5312.08193 HOMO: -7.85865 LUMO: 2.83543 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.10780 HOMO: -6.78924 LUMO: 2.42181 factor:1 | 1 (-0.66018) | -1 | -1 |
| G: -5312.08193 HOMO: -7.85865 LUMO: 2.83543 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.96911 HOMO: -6.94707 LUMO: 1.71704 factor:1 | 1 (-0.52148) | -1 | -1 |
| G: -5312.08193 HOMO: -7.85865 LUMO: 2.83543 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.01485 HOMO: -6.85183 LUMO: 1.78779 factor:1 | 1 (-0.56722) | -1 | -1 |
| G: -5312.08193 HOMO: -7.85865 LUMO: 2.83543 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.94728 HOMO: -6.98788 LUMO: 1.69799 factor:1 | 1 (-0.49966) | -1 | -1 |
| G: -5312.08193 HOMO: -7.85865 LUMO: 2.83543 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.91156 HOMO: -6.79468 LUMO: 2.04358 factor:1 | 1 (-0.46393) | -1 | -1 |
| G: -5312.08193 HOMO: -7.85865 LUMO: 2.83543 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.79046 HOMO: -6.90081 LUMO: 1.97283 factor:1 | 1 (-0.34284) | -1 | -1 |
| G: -5312.08193 HOMO: -7.85865 LUMO: 2.83543 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.98707 HOMO: -6.79468 LUMO: 2.00820 factor:1 | 1 (-0.53944) | -1 | -1 |
| G: -5312.08193 HOMO: -7.85865 LUMO: 2.83543 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.87191 HOMO: -7.06408 LUMO: 2.29936 factor:1 | 1 (-0.42428) | -1 | -1 |
| G: -5312.08193 HOMO: -7.85865 LUMO: 2.83543 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.15814 HOMO: -6.78924 LUMO: 2.13337 factor:1 | 1 (-0.71052) | -1 | -1 |
| G: -5312.08193 HOMO: -7.85865 LUMO: 2.83543 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.97226 HOMO: -6.79468 LUMO: 2.35106 factor:1 | 1 (-0.52464) | -1 | -1 |
| G: -5312.08193 HOMO: -7.85865 LUMO: 2.83543 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.93123 HOMO: -6.82734 LUMO: 2.16603 factor:1 | 1 (-0.48360) | -1 | -1 |
| G: -5312.08193 HOMO: -7.85865 LUMO: 2.83543 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.89789 HOMO: -6.79740 LUMO: 2.36739 factor:1 | 1 (-0.45027) | -1 | -1 |
| G: -5312.08193 HOMO: -7.85865 LUMO: 2.83543 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.04990 HOMO: -7.14027 LUMO: 2.10888 factor:1 | 1 (-0.60227) | -1 | -1 |
| G: -5312.08193 HOMO: -6.61509 LUMO: -0.23674 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.78608 HOMO: -6.96067 LUMO: 1.59731 factor:1 | 1 (-0.33846) | -1 | -1 |
| G: -5312.08193 HOMO: -6.61509 LUMO: -0.23674 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.96845 HOMO: -6.91169 LUMO: 1.37145 factor:1 | 1 (-0.52083) | -1 | -1 |
| G: -5312.08193 HOMO: -6.61509 LUMO: -0.23674 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.77359 HOMO: -6.94707 LUMO: 1.73064 factor:1 | 1 (-0.32597) | -1 | -1 |
| G: -5312.08193 HOMO: -6.61509 LUMO: -0.23674 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.96737 HOMO: -7.02326 LUMO: 1.41227 factor:1 | 1 (-0.51974) | -1 | -1 |
| G: -5312.08193 HOMO: -6.61509 LUMO: -0.23674 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.77528 HOMO: -6.72121 LUMO: 1.43132 factor:1 | 1 (-0.32765) | -1 | -1 |
| G: -5312.08193 HOMO: -6.61509 LUMO: -0.23674 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.98138 HOMO: -6.51168 LUMO: 1.72520 factor:1 | 1 (-0.53375) | -1 | -1 |
| G: -5312.08193 HOMO: -6.61509 LUMO: -0.23674 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.81403 HOMO: -6.98516 LUMO: 1.92929 factor:1 | 1 (-0.36640) | -1 | -1 |
| G: -5312.08193 HOMO: -6.61509 LUMO: -0.23674 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.43704 HOMO: -6.92802 LUMO: 2.07895 factor:1 | -1 (0.01059) | -1 | -1 |
| G: -5312.08193 HOMO: -6.61509 LUMO: -0.23674 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.65620 HOMO: -7.02326 LUMO: 1.86398 factor:1 | 1 (-0.20858) | -1 | -1 |
| G: -5312.08193 HOMO: -6.61509 LUMO: -0.23674 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.51533 HOMO: -6.82462 LUMO: 1.86670 factor:1 | 1 (-0.06770) | -1 | -1 |
| G: -5312.08193 HOMO: -6.61509 LUMO: -0.23674 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.85691 HOMO: -6.83278 LUMO: 1.71160 factor:1 | 1 (-0.40929) | -1 | -1 |
| G: -5312.08193 HOMO: -6.61509 LUMO: -0.23674 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.58203 HOMO: -6.62869 LUMO: 1.69527 factor:1 | 1 (-0.13440) | -1 | -1 |
| G: -5312.08193 HOMO: -6.61509 LUMO: -0.23674 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.54646 HOMO: -6.84094 LUMO: 1.27349 factor:1 | 1 (-0.09883) | -1 | -1 |
| G: -5312.08193 HOMO: -6.61509 LUMO: -0.23674 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.38580 HOMO: -7.07768 LUMO: 1.27621 factor:1 | -1 (0.06182) | 1 | -1 |
| G: -5312.08193 HOMO: -6.61509 LUMO: -0.23674 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.73158 HOMO: -7.06135 LUMO: 1.55105 factor:1 | 1 (-0.28395) | 1 | -1 |
| G: -5312.08193 HOMO: -6.61509 LUMO: -0.23674 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.91675 HOMO: -6.94162 LUMO: 1.64629 factor:1 | 1 (-0.46912) | -1 | -1 |
| G: -5312.08193 HOMO: -6.61509 LUMO: -0.23674 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.91068 HOMO: -7.07224 LUMO: 1.65445 factor:1 | 1 (-0.46306) | 1 | -1 |
| G: -5312.08193 HOMO: -6.61509 LUMO: -0.23674 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.89278 HOMO: -6.68584 LUMO: 1.91296 factor:1 | 1 (-0.44515) | -1 | -1 |
| G: -5312.08193 HOMO: -6.61509 LUMO: -0.23674 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.01104 HOMO: -7.09129 LUMO: 1.73609 factor:1 | 1 (-0.56341) | 1 | -1 |
| G: -5312.08193 HOMO: -6.61509 LUMO: -0.23674 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.03980 HOMO: -7.01237 LUMO: 2.01092 factor:1 | 1 (-0.59217) | -1 | -1 |
| G: -5312.08193 HOMO: -6.61509 LUMO: -0.23674 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.92524 HOMO: -6.93618 LUMO: 1.63540 factor:1 | 1 (-0.47761) | -1 | -1 |
| G: -5312.08193 HOMO: -6.61509 LUMO: -0.23674 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.88745 HOMO: -6.98516 LUMO: 1.64629 factor:1 | 1 (-0.43982) | -1 | -1 |
| G: -5312.08193 HOMO: -6.61509 LUMO: -0.23674 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.84663 HOMO: -6.80285 LUMO: 1.95106 factor:1 | 1 (-0.39900) | -1 | -1 |
| G: -5312.08193 HOMO: -6.61509 LUMO: -0.23674 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.82842 HOMO: -6.76747 LUMO: 1.88303 factor:1 | 1 (-0.38080) | -1 | -1 |
| G: -5312.08193 HOMO: -6.61509 LUMO: -0.23674 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.72116 HOMO: -6.64230 LUMO: 1.90480 factor:1 | 1 (-0.27353) | -1 | -1 |
| G: -5312.08193 HOMO: -6.61509 LUMO: -0.23674 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.69435 HOMO: -6.93618 LUMO: 2.19324 factor:1 | 1 (-0.24673) | -1 | -1 |
| G: -5312.08193 HOMO: -6.61509 LUMO: -0.23674 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.71814 HOMO: -6.95523 LUMO: 1.80684 factor:1 | 1 (-0.27051) | -1 | -1 |
| G: -5312.08193 HOMO: -6.61509 LUMO: -0.23674 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.92380 HOMO: -6.66135 LUMO: 1.72792 factor:1 | 1 (-0.47617) | -1 | -1 |
| G: -5312.08193 HOMO: -6.61509 LUMO: -0.23674 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.67005 HOMO: -6.36202 LUMO: 1.89391 factor:1 | 1 (-1.22242) | -1 | -1 |
| G: -5312.08193 HOMO: -6.61509 LUMO: -0.23674 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.79258 HOMO: -7.03959 LUMO: 2.06262 factor:1 | 1 (-1.34495) | -1 | -1 |
| G: -5312.08193 HOMO: -6.61509 LUMO: -0.23674 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.86420 HOMO: -7.08584 LUMO: 2.01092 factor:1 | 1 (-1.41657) | 1 | -1 |
| G: -5312.08193 HOMO: -6.80285 LUMO: -0.55783 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.47829 HOMO: -6.96067 LUMO: 1.59731 factor:1 | 1 (-1.03066) | -1 | -1 |
| G: -5312.08193 HOMO: -6.80285 LUMO: -0.55783 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.43505 HOMO: -6.91169 LUMO: 1.37145 factor:1 | 1 (-0.98742) | -1 | -1 |
| G: -5312.08193 HOMO: -6.80285 LUMO: -0.55783 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.44961 HOMO: -6.94707 LUMO: 1.73064 factor:1 | 1 (-1.00198) | -1 | -1 |
| G: -5312.08193 HOMO: -6.80285 LUMO: -0.55783 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.43265 HOMO: -7.02326 LUMO: 1.41227 factor:1 | 1 (-0.98502) | -1 | -1 |
| G: -5312.08193 HOMO: -6.80285 LUMO: -0.55783 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.28158 HOMO: -6.72121 LUMO: 1.43132 factor:1 | 1 (-0.83395) | -1 | -1 |
| G: -5312.08193 HOMO: -6.80285 LUMO: -0.55783 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.62134 HOMO: -6.51168 LUMO: 1.72520 factor:1 | 1 (-1.17371) | -1 | -1 |
| G: -5312.08193 HOMO: -6.80285 LUMO: -0.55783 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.47763 HOMO: -6.98516 LUMO: 1.92929 factor:1 | 1 (-1.03001) | -1 | -1 |
| G: -5312.08193 HOMO: -6.80285 LUMO: -0.55783 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.59516 HOMO: -6.92802 LUMO: 2.07895 factor:1 | 1 (-1.14753) | -1 | -1 |
| G: -5312.08193 HOMO: -6.80285 LUMO: -0.55783 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11578.21272 HOMO: -7.02326 LUMO: 1.86398 factor:1 | 1 (-1.76509) | -1 | -1 |
| G: -5312.08193 HOMO: -6.80285 LUMO: -0.55783 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11578.00401 HOMO: -6.82462 LUMO: 1.86670 factor:1 | 1 (-1.55638) | -1 | -1 |
| G: -5312.08193 HOMO: -6.80285 LUMO: -0.55783 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11578.02303 HOMO: -6.83278 LUMO: 1.71160 factor:1 | 1 (-1.57540) | -1 | -1 |
| G: -5312.08193 HOMO: -6.80285 LUMO: -0.55783 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11578.83529 HOMO: -6.62869 LUMO: 1.69527 factor:1 | 1 (-2.38766) | -1 | -1 |
| G: -5312.08193 HOMO: -6.80285 LUMO: -0.55783 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11578.98079 HOMO: -6.84094 LUMO: 1.27349 factor:1 | 1 (-2.53316) | -1 | -1 |
| G: -5312.08193 HOMO: -6.80285 LUMO: -0.55783 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.97506 HOMO: -7.07768 LUMO: 1.27621 factor:1 | 1 (-1.52743) | 1 | -1 |
| G: -5312.08193 HOMO: -6.80285 LUMO: -0.55783 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11578.15620 HOMO: -7.06135 LUMO: 1.55105 factor:1 | 1 (-1.70858) | 1 | -1 |
| G: -5312.08193 HOMO: -6.80285 LUMO: -0.55783 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.79141 HOMO: -6.94162 LUMO: 1.64629 factor:1 | 1 (-1.34378) | -1 | -1 |
| G: -5312.08193 HOMO: -6.80285 LUMO: -0.55783 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11578.04156 HOMO: -7.07224 LUMO: 1.65445 factor:1 | 1 (-1.59393) | 1 | -1 |
| G: -5312.08193 HOMO: -6.80285 LUMO: -0.55783 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.78665 HOMO: -6.68584 LUMO: 1.91296 factor:1 | 1 (-1.33902) | -1 | -1 |
| G: -5312.08193 HOMO: -6.80285 LUMO: -0.55783 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.80286 HOMO: -7.09129 LUMO: 1.73609 factor:1 | 1 (-1.35524) | 1 | -1 |
| G: -5312.08193 HOMO: -6.80285 LUMO: -0.55783 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.73818 HOMO: -7.01237 LUMO: 2.01092 factor:1 | 1 (-1.29055) | -1 | -1 |
| G: -5312.08193 HOMO: -6.80285 LUMO: -0.55783 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.59813 HOMO: -6.93618 LUMO: 1.63540 factor:1 | 1 (-1.15050) | -1 | -1 |
| G: -5312.08193 HOMO: -6.80285 LUMO: -0.55783 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.75245 HOMO: -6.98516 LUMO: 1.64629 factor:1 | 1 (-0.30482) | -1 | -1 |
| G: -5312.08193 HOMO: -6.80285 LUMO: -0.55783 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.96494 HOMO: -6.80285 LUMO: 1.95106 factor:1 | 1 (-0.51732) | -1 | -1 |
| G: -5312.08193 HOMO: -6.80285 LUMO: -0.55783 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.84187 HOMO: -6.76747 LUMO: 1.88303 factor:1 | 1 (-0.39424) | -1 | -1 |
| G: -5312.08193 HOMO: -6.80285 LUMO: -0.55783 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.90619 HOMO: -6.64230 LUMO: 1.90480 factor:1 | 1 (-0.45857) | -1 | -1 |
| G: -5312.08193 HOMO: -6.80285 LUMO: -0.55783 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.92399 HOMO: -6.93618 LUMO: 2.19324 factor:1 | 1 (-0.47636) | -1 | -1 |
| G: -5312.08193 HOMO: -6.80285 LUMO: -0.55783 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.91158 HOMO: -6.95523 LUMO: 1.80684 factor:1 | 1 (-0.46395) | -1 | -1 |
| G: -5312.08193 HOMO: -6.80285 LUMO: -0.55783 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.82829 HOMO: -6.66135 LUMO: 1.72792 factor:1 | 1 (-0.38066) | -1 | -1 |
| G: -5312.08193 HOMO: -6.80285 LUMO: -0.55783 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.77049 HOMO: -6.36202 LUMO: 1.89391 factor:1 | 1 (-0.32286) | -1 | -1 |
| G: -5312.08193 HOMO: -6.80285 LUMO: -0.55783 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.73539 HOMO: -7.03959 LUMO: 2.06262 factor:1 | 1 (-0.28776) | -1 | -1 |
| G: -5312.08193 HOMO: -6.80285 LUMO: -0.55783 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.56192 HOMO: -7.08584 LUMO: 2.01092 factor:1 | 1 (-0.11429) | 1 | -1 |
| G: -5312.08193 HOMO: -7.16476 LUMO: 2.86264 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.92170 HOMO: -6.96067 LUMO: 1.59731 factor:1 | 1 (-0.47408) | -1 | -1 |
| G: -5312.08193 HOMO: -7.16476 LUMO: 2.86264 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.75297 HOMO: -6.91169 LUMO: 1.37145 factor:1 | 1 (-0.30534) | -1 | -1 |
| G: -5312.08193 HOMO: -7.16476 LUMO: 2.86264 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.69699 HOMO: -6.94707 LUMO: 1.73064 factor:1 | 1 (-0.24937) | -1 | -1 |
| G: -5312.08193 HOMO: -7.16476 LUMO: 2.86264 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.98160 HOMO: -7.02326 LUMO: 1.41227 factor:1 | 1 (-0.53397) | -1 | -1 |
| G: -5312.08193 HOMO: -7.16476 LUMO: 2.86264 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.72401 HOMO: -6.72121 LUMO: 1.43132 factor:1 | 1 (-0.27639) | -1 | -1 |
| G: -5312.08193 HOMO: -7.16476 LUMO: 2.86264 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.75727 HOMO: -6.51168 LUMO: 1.72520 factor:1 | 1 (-0.30964) | -1 | -1 |
| G: -5312.08193 HOMO: -7.16476 LUMO: 2.86264 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.85528 HOMO: -6.98516 LUMO: 1.92929 factor:1 | 1 (-0.40765) | -1 | -1 |
| G: -5312.08193 HOMO: -7.16476 LUMO: 2.86264 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.76763 HOMO: -6.92802 LUMO: 2.07895 factor:1 | 1 (-0.32001) | -1 | -1 |
| G: -5312.08193 HOMO: -7.16476 LUMO: 2.86264 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.92845 HOMO: -7.02326 LUMO: 1.86398 factor:1 | 1 (-0.48083) | -1 | -1 |
| G: -5312.08193 HOMO: -7.16476 LUMO: 2.86264 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.62467 HOMO: -6.82462 LUMO: 1.86670 factor:1 | 1 (-0.17704) | -1 | -1 |
| G: -5312.08193 HOMO: -7.16476 LUMO: 2.86264 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.77778 HOMO: -6.83278 LUMO: 1.71160 factor:1 | 1 (-0.33016) | -1 | -1 |
| G: -5312.08193 HOMO: -7.16476 LUMO: 2.86264 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.50012 HOMO: -6.62869 LUMO: 1.69527 factor:1 | 1 (-0.05249) | -1 | -1 |
| G: -5312.08193 HOMO: -7.16476 LUMO: 2.86264 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.82051 HOMO: -6.84094 LUMO: 1.27349 factor:1 | 1 (-0.37288) | -1 | -1 |
| G: -5312.08193 HOMO: -7.16476 LUMO: 2.86264 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.71103 HOMO: -7.07768 LUMO: 1.27621 factor:1 | 1 (-0.26341) | -1 | -1 |
| G: -5312.08193 HOMO: -7.16476 LUMO: 2.86264 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.78891 HOMO: -7.06135 LUMO: 1.55105 factor:1 | 1 (-0.34129) | -1 | -1 |
| G: -5312.08193 HOMO: -7.16476 LUMO: 2.86264 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.69014 HOMO: -6.94162 LUMO: 1.64629 factor:1 | 1 (-0.24251) | -1 | -1 |
| G: -5312.08193 HOMO: -7.16476 LUMO: 2.86264 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.82894 HOMO: -7.07224 LUMO: 1.65445 factor:1 | 1 (-0.38131) | -1 | -1 |
| G: -5312.08193 HOMO: -7.16476 LUMO: 2.86264 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.67944 HOMO: -6.68584 LUMO: 1.91296 factor:1 | 1 (-0.23181) | -1 | -1 |
| G: -5312.08193 HOMO: -7.16476 LUMO: 2.86264 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.68910 HOMO: -7.09129 LUMO: 1.73609 factor:1 | 1 (-0.24147) | -1 | -1 |
| G: -5312.08193 HOMO: -7.16476 LUMO: 2.86264 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.54450 HOMO: -7.01237 LUMO: 2.01092 factor:1 | 1 (-0.09687) | -1 | -1 |
| G: -5312.08193 HOMO: -7.16476 LUMO: 2.86264 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.59109 HOMO: -6.93618 LUMO: 1.63540 factor:1 | 1 (-0.14346) | -1 | -1 |
| G: -5312.08193 HOMO: -7.16476 LUMO: 2.86264 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.88883 HOMO: -6.98516 LUMO: 1.64629 factor:1 | 1 (-0.44121) | -1 | -1 |
| G: -5312.08193 HOMO: -7.16476 LUMO: 2.86264 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.73686 HOMO: -6.80285 LUMO: 1.95106 factor:1 | 1 (-0.28923) | -1 | -1 |
| G: -5312.08193 HOMO: -7.16476 LUMO: 2.86264 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.79438 HOMO: -6.76747 LUMO: 1.88303 factor:1 | 1 (-0.34675) | -1 | -1 |
| G: -5312.08193 HOMO: -7.16476 LUMO: 2.86264 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.79302 HOMO: -6.64230 LUMO: 1.90480 factor:1 | 1 (-0.34539) | -1 | -1 |
| G: -5312.08193 HOMO: -7.16476 LUMO: 2.86264 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11578.18801 HOMO: -6.93618 LUMO: 2.19324 factor:1 | 1 (-1.74039) | -1 | -1 |
| G: -5312.08193 HOMO: -7.16476 LUMO: 2.86264 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11578.97167 HOMO: -6.95523 LUMO: 1.80684 factor:1 | 1 (-2.52405) | -1 | -1 |
| G: -5312.08193 HOMO: -7.16476 LUMO: 2.86264 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.98662 HOMO: -6.66135 LUMO: 1.72792 factor:1 | 1 (-1.53899) | -1 | -1 |
| G: -5312.08193 HOMO: -7.16476 LUMO: 2.86264 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11578.13373 HOMO: -6.36202 LUMO: 1.89391 factor:1 | 1 (-1.68610) | -1 | -1 |
| G: -5312.08193 HOMO: -7.16476 LUMO: 2.86264 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11578.14733 HOMO: -7.03959 LUMO: 2.06262 factor:1 | 1 (-1.69970) | -1 | -1 |
| G: -5312.08193 HOMO: -7.16476 LUMO: 2.86264 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11578.00404 HOMO: -7.08584 LUMO: 2.01092 factor:1 | 1 (-1.55641) | -1 | -1 |
| G: -5312.08193 HOMO: -6.50352 LUMO: 2.10888 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.68978 HOMO: -6.96067 LUMO: 1.59731 factor:1 | 1 (-0.24215) | 1 | 1 |
| G: -5312.08193 HOMO: -6.50352 LUMO: 2.10888 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.74864 HOMO: -6.91169 LUMO: 1.37145 factor:1 | 1 (-0.30101) | -1 | -1 |
| G: -5312.08193 HOMO: -6.50352 LUMO: 2.10888 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.75269 HOMO: -6.94707 LUMO: 1.73064 factor:1 | 1 (-0.30507) | 1 | 1 |
| G: -5312.08193 HOMO: -6.50352 LUMO: 2.10888 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.55775 HOMO: -7.02326 LUMO: 1.41227 factor:1 | 1 (-0.11012) | -1 | -1 |
| G: -5312.08193 HOMO: -6.50352 LUMO: 2.10888 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.61917 HOMO: -6.72121 LUMO: 1.43132 factor:1 | 1 (-0.17154) | -1 | -1 |
| G: -5312.08193 HOMO: -6.50352 LUMO: 2.10888 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.43552 HOMO: -6.51168 LUMO: 1.72520 factor:1 | -1 (0.01211) | 1 | 1 |
| G: -5312.08193 HOMO: -6.50352 LUMO: 2.10888 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.42877 HOMO: -6.98516 LUMO: 1.92929 factor:1 | -1 (0.01886) | 1 | 1 |
| G: -5312.08193 HOMO: -6.50352 LUMO: 2.10888 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.81506 HOMO: -6.92802 LUMO: 2.07895 factor:1 | 1 (-0.36744) | 1 | 1 |
| G: -5312.08193 HOMO: -6.50352 LUMO: 2.10888 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.65373 HOMO: -7.02326 LUMO: 1.86398 factor:1 | 1 (-0.20610) | 1 | 1 |
| G: -5312.08193 HOMO: -6.50352 LUMO: 2.10888 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.64442 HOMO: -6.82462 LUMO: 1.86670 factor:1 | 1 (-0.19679) | 1 | 1 |
| G: -5312.08193 HOMO: -6.50352 LUMO: 2.10888 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.74826 HOMO: -6.83278 LUMO: 1.71160 factor:1 | 1 (-0.30063) | 1 | 1 |
| G: -5312.08193 HOMO: -6.50352 LUMO: 2.10888 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11578.46035 HOMO: -6.62869 LUMO: 1.69527 factor:1 | 1 (-2.01272) | 1 | 1 |
| G: -5312.08193 HOMO: -6.50352 LUMO: 2.10888 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.67075 HOMO: -6.84094 LUMO: 1.27349 factor:1 | 1 (-1.22312) | -1 | -1 |
| G: -5312.08193 HOMO: -6.50352 LUMO: 2.10888 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.71456 HOMO: -7.07768 LUMO: 1.27621 factor:1 | 1 (-1.26693) | -1 | -1 |
| G: -5312.08193 HOMO: -6.50352 LUMO: 2.10888 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.74607 HOMO: -7.06135 LUMO: 1.55105 factor:1 | 1 (-1.29845) | -1 | -1 |
| G: -5312.08193 HOMO: -6.50352 LUMO: 2.10888 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.74722 HOMO: -6.94162 LUMO: 1.64629 factor:1 | 1 (-1.29959) | 1 | 1 |
| G: -5312.08193 HOMO: -6.50352 LUMO: 2.10888 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.60368 HOMO: -7.07224 LUMO: 1.65445 factor:1 | 1 (-1.15605) | 1 | 1 |
| G: -5312.08193 HOMO: -6.50352 LUMO: 2.10888 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.80047 HOMO: -6.68584 LUMO: 1.91296 factor:1 | 1 (-1.35284) | 1 | 1 |
| G: -5313.11806 HOMO: -6.50352 LUMO: 2.10888 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.03352 HOMO: -7.09129 LUMO: 1.73609 factor:1 | -1 (0.45024) | 1 | 1 |
| G: -5313.11806 HOMO: -6.50352 LUMO: 2.10888 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.84902 HOMO: -7.01237 LUMO: 2.01092 factor:1 | -1 (0.63473) | 1 | 1 |
| G: -5313.11806 HOMO: -6.50352 LUMO: 2.10888 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.57944 HOMO: -6.93618 LUMO: 1.63540 factor:1 | -1 (0.90432) | 1 | 1 |
| G: -5313.11806 HOMO: -6.50352 LUMO: 2.10888 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11578.44220 HOMO: -6.98516 LUMO: 1.64629 factor:1 | 1 (-0.95844) | 1 | 1 |
| G: -5313.11806 HOMO: -6.50352 LUMO: 2.10888 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11578.06807 HOMO: -6.80285 LUMO: 1.95106 factor:1 | 1 (-0.58431) | 1 | 1 |
| G: -5313.11806 HOMO: -6.50352 LUMO: 2.10888 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11579.01581 HOMO: -6.76747 LUMO: 1.88303 factor:1 | 1 (-1.53206) | 1 | 1 |
| G: -5313.11806 HOMO: -6.50352 LUMO: 2.10888 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11578.14426 HOMO: -6.64230 LUMO: 1.90480 factor:1 | 1 (-0.66050) | 1 | 1 |
| G: -5313.11806 HOMO: -6.50352 LUMO: 2.10888 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11578.29803 HOMO: -6.93618 LUMO: 2.19324 factor:1 | 1 (-0.81427) | 1 | 1 |
| G: -5313.11806 HOMO: -6.50352 LUMO: 2.10888 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.87095 HOMO: -6.95523 LUMO: 1.80684 factor:1 | 1 (-0.38719) | 1 | 1 |
| G: -5313.11806 HOMO: -6.50352 LUMO: 2.10888 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.91870 HOMO: -6.66135 LUMO: 1.72792 factor:1 | 1 (-0.43495) | 1 | 1 |
| G: -5313.11806 HOMO: -6.50352 LUMO: 2.10888 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.90734 HOMO: -6.36202 LUMO: 1.89391 factor:1 | -1 (0.57642) | -1 | -1 |
| G: -5313.11806 HOMO: -6.50352 LUMO: 2.10888 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.31279 HOMO: -7.03959 LUMO: 2.06262 factor:1 | -1 (0.17097) | 1 | 1 |
| G: -5313.11806 HOMO: -6.50352 LUMO: 2.10888 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.94470 HOMO: -7.08584 LUMO: 2.01092 factor:1 | -1 (0.53906) | 1 | 1 |
| G: -5313.11806 HOMO: -6.59604 LUMO: 2.33746 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.26729 HOMO: -6.96067 LUMO: 1.59731 factor:1 | -1 (0.21647) | 1 | 1 |
| G: -5313.11806 HOMO: -6.59604 LUMO: 2.33746 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.20982 HOMO: -6.91169 LUMO: 1.37145 factor:1 | -1 (0.27394) | -1 | -1 |
| G: -5313.11806 HOMO: -6.59604 LUMO: 2.33746 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.44933 HOMO: -6.94707 LUMO: 1.73064 factor:1 | -1 (0.03442) | 1 | 1 |
| G: -5313.11806 HOMO: -6.59604 LUMO: 2.33746 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.61638 HOMO: -7.02326 LUMO: 1.41227 factor:1 | 1 (-0.13263) | -1 | -1 |
| G: -5313.11806 HOMO: -6.59604 LUMO: 2.33746 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.80545 HOMO: -6.72121 LUMO: 1.43132 factor:1 | 1 (-0.32169) | -1 | -1 |
| G: -5313.11806 HOMO: -6.59604 LUMO: 2.33746 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.94529 HOMO: -6.51168 LUMO: 1.72520 factor:1 | 1 (-0.46153) | -1 | -1 |
| G: -5313.11806 HOMO: -6.59604 LUMO: 2.33746 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.65973 HOMO: -6.98516 LUMO: 1.92929 factor:1 | 1 (-0.17598) | 1 | 1 |
| G: -5313.11806 HOMO: -6.59604 LUMO: 2.33746 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.23591 HOMO: -6.92802 LUMO: 2.07895 factor:1 | -1 (0.24784) | 1 | 1 |
| G: -5313.11806 HOMO: -6.59604 LUMO: 2.33746 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.16650 HOMO: -7.02326 LUMO: 1.86398 factor:1 | -1 (0.31726) | 1 | 1 |
| G: -5313.11806 HOMO: -6.59604 LUMO: 2.33746 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.81999 HOMO: -6.82462 LUMO: 1.86670 factor:1 | -1 (0.66377) | 1 | 1 |
| G: -5313.11806 HOMO: -6.59604 LUMO: 2.33746 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.19684 HOMO: -6.83278 LUMO: 1.71160 factor:1 | -1 (0.28692) | 1 | 1 |
| G: -5313.11806 HOMO: -6.59604 LUMO: 2.33746 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.95011 HOMO: -6.62869 LUMO: 1.69527 factor:1 | -1 (0.53364) | 1 | 1 |
| G: -5313.11806 HOMO: -6.59604 LUMO: 2.33746 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.75980 HOMO: -6.84094 LUMO: 1.27349 factor:1 | -1 (0.72396) | -1 | -1 |
| G: -5313.11806 HOMO: -6.59604 LUMO: 2.33746 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.04078 HOMO: -7.07768 LUMO: 1.27621 factor:1 | -1 (0.44297) | -1 | -1 |
| G: -5313.11806 HOMO: -6.59604 LUMO: 2.33746 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.98805 HOMO: -7.06135 LUMO: 1.55105 factor:1 | -1 (0.49571) | -1 | -1 |
| G: -5313.11806 HOMO: -6.59604 LUMO: 2.33746 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11578.40693 HOMO: -6.94162 LUMO: 1.64629 factor:1 | 1 (-0.92317) | 1 | 1 |
| G: -5313.11806 HOMO: -6.59604 LUMO: 2.33746 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.71807 HOMO: -7.07224 LUMO: 1.65445 factor:1 | 1 (-0.23432) | 1 | 1 |
| G: -5313.11806 HOMO: -6.59604 LUMO: 2.33746 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.81658 HOMO: -6.68584 LUMO: 1.91296 factor:1 | 1 (-0.33282) | 1 | 1 |
| G: -5313.11806 HOMO: -6.59604 LUMO: 2.33746 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11578.02926 HOMO: -7.09129 LUMO: 1.73609 factor:1 | 1 (-0.54551) | 1 | 1 |
| G: -5313.11806 HOMO: -6.59604 LUMO: 2.33746 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11578.34372 HOMO: -7.01237 LUMO: 2.01092 factor:1 | 1 (-0.85996) | 1 | 1 |
| G: -5313.11806 HOMO: -6.59604 LUMO: 2.33746 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11578.21977 HOMO: -6.93618 LUMO: 1.63540 factor:1 | 1 (-0.73601) | 1 | 1 |
| G: -5313.11806 HOMO: -6.59604 LUMO: 2.33746 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11578.26497 HOMO: -6.98516 LUMO: 1.64629 factor:1 | 1 (-0.78121) | 1 | 1 |
| G: -5313.11806 HOMO: -6.59604 LUMO: 2.33746 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11578.14668 HOMO: -6.80285 LUMO: 1.95106 factor:1 | 1 (-0.66292) | 1 | 1 |
| G: -5313.11806 HOMO: -6.59604 LUMO: 2.33746 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.03763 HOMO: -6.76747 LUMO: 1.88303 factor:1 | -1 (0.44613) | 1 | 1 |
| G: -5313.11806 HOMO: -6.59604 LUMO: 2.33746 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.87120 HOMO: -6.64230 LUMO: 1.90480 factor:1 | -1 (0.61256) | 1 | 1 |
| G: -5313.11806 HOMO: -6.59604 LUMO: 2.33746 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.07972 HOMO: -6.93618 LUMO: 2.19324 factor:1 | -1 (0.40403) | 1 | 1 |
| G: -5313.11806 HOMO: -6.59604 LUMO: 2.33746 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11578.43659 HOMO: -6.95523 LUMO: 1.80684 factor:1 | 1 (-0.95283) | 1 | 1 |
| G: -5313.11806 HOMO: -6.59604 LUMO: 2.33746 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.90921 HOMO: -6.66135 LUMO: 1.72792 factor:1 | 1 (-0.42545) | 1 | 1 |
| G: -5313.11806 HOMO: -6.59604 LUMO: 2.33746 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.80221 HOMO: -6.36202 LUMO: 1.89391 factor:1 | 1 (-0.31845) | -1 | -1 |
| G: -5313.11806 HOMO: -6.59604 LUMO: 2.33746 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.90619 HOMO: -7.03959 LUMO: 2.06262 factor:1 | 1 (-0.42243) | 1 | 1 |
| G: -5313.11806 HOMO: -6.59604 LUMO: 2.33746 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11578.00703 HOMO: -7.08584 LUMO: 2.01092 factor:1 | 1 (-0.52327) | 1 | 1 |
| G: -5313.11806 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.87946 HOMO: -7.06135 LUMO: 0.75376 factor:1 | 1 (-0.39571) | 1 | -1 |
| G: -5313.11806 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.13657 HOMO: -5.10213 LUMO: 0.77825 factor:1 | -1 (0.34719) | -1 | -1 |
| G: -5313.11806 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.05120 HOMO: -5.84228 LUMO: 0.50341 factor:1 | -1 (0.43255) | -1 | -1 |
| G: -5313.11806 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.94410 HOMO: -5.39874 LUMO: 0.68028 factor:1 | -1 (0.53966) | -1 | -1 |
| G: -5313.11806 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.12138 HOMO: -5.16744 LUMO: 1.14832 factor:1 | -1 (0.36237) | -1 | -1 |
| G: -5313.11806 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.04282 HOMO: -5.80963 LUMO: 0.35647 factor:1 | -1 (0.44093) | -1 | -1 |
| G: -5313.11806 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.03874 HOMO: -5.02322 LUMO: 1.07213 factor:1 | -1 (0.44502) | -1 | -1 |
| G: -5313.11806 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.05523 HOMO: -5.80963 LUMO: 0.56328 factor:1 | -1 (0.42852) | -1 | -1 |
| G: -5313.11806 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.92949 HOMO: -5.45316 LUMO: 0.78369 factor:1 | -1 (0.55427) | -1 | -1 |
| G: -5313.11806 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.12590 HOMO: -5.25452 LUMO: 0.82178 factor:1 | -1 (0.35786) | -1 | -1 |
| G: -5313.11806 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.08603 HOMO: -5.21370 LUMO: 1.03947 factor:1 | -1 (0.39772) | -1 | -1 |
| G: -5313.11806 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.07700 HOMO: -6.04365 LUMO: 0.31837 factor:1 | -1 (0.40676) | -1 | -1 |
| G: -5313.11806 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.84032 HOMO: -5.86405 LUMO: 0.55511 factor:1 | -1 (0.64344) | -1 | -1 |
| G: -5313.11806 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.02666 HOMO: -5.64908 LUMO: 0.71022 factor:1 | -1 (0.45710) | -1 | -1 |
| G: -5313.11806 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.85101 HOMO: -5.94297 LUMO: 0.68301 factor:1 | -1 (0.63275) | -1 | -1 |
| G: -5313.11806 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.06329 HOMO: -6.01916 LUMO: 0.56328 factor:1 | -1 (0.42047) | -1 | -1 |
| G: -5313.11806 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11579.05184 HOMO: -6.05181 LUMO: 0.35103 factor:1 | 1 (-1.56808) | -1 | -1 |
| G: -5313.11806 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11578.24889 HOMO: -6.08447 LUMO: 0.48436 factor:1 | 1 (-0.76513) | -1 | -1 |
| G: -5313.11806 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11578.30391 HOMO: -5.86950 LUMO: 0.36735 factor:1 | 1 (-0.82015) | -1 | -1 |
| G: -5313.11806 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.91966 HOMO: -5.33615 LUMO: 0.65852 factor:1 | -1 (0.56409) | -1 | -1 |
| G: -5313.11806 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.90990 HOMO: -5.36064 LUMO: 0.86804 factor:1 | -1 (0.57386) | -1 | -1 |
| G: -5313.11806 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.92821 HOMO: -5.74160 LUMO: 0.64491 factor:1 | -1 (0.55555) | -1 | -1 |
| G: -5313.11806 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.01300 HOMO: -5.23003 LUMO: 0.66124 factor:1 | -1 (0.47076) | -1 | -1 |
| G: -5313.11806 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11578.36530 HOMO: -5.77698 LUMO: 0.84083 factor:1 | 1 (-0.88154) | -1 | -1 |
| G: -5313.11806 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.72863 HOMO: -5.60555 LUMO: 0.84355 factor:1 | 1 (-0.24488) | -1 | -1 |
| G: -5313.11806 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.93634 HOMO: -7.11578 LUMO: -1.62452 factor:1 | 1 (-0.45258) | -1 | -1 |
| G: -5313.11806 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.90281 HOMO: -7.23279 LUMO: -1.63813 factor:1 | 1 (-0.41906) | -1 | -1 |
| G: -5313.11806 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.89751 HOMO: -6.68312 LUMO: -0.88709 factor:1 | 1 (-0.41375) | -1 | -1 |
| G: -5313.11806 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.93692 HOMO: -6.99333 LUMO: -0.88709 factor:1 | -1 (0.54684) | -1 | -1 |
| G: -5313.11806 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.06900 HOMO: -7.40694 LUMO: 0.11973 factor:1 | -1 (0.41476) | 1 | 1 |
| G: -5313.11806 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.92396 HOMO: -6.74026 LUMO: -0.72927 factor:1 | -1 (0.55979) | -1 | -1 |
| G: -5313.11806 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.15140 HOMO: -6.67223 LUMO: -0.70750 factor:1 | -1 (0.33236) | -1 | -1 |
| G: -5313.11806 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.18797 HOMO: -7.06952 LUMO: -1.40139 factor:1 | -1 (0.29579) | -1 | -1 |
| G: -5313.11806 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.46615 HOMO: -7.21374 LUMO: -1.13199 factor:1 | -1 (0.01761) | -1 | -1 |
| G: -5313.11806 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.13589 HOMO: -6.54706 LUMO: -1.34424 factor:1 | -1 (0.34787) | -1 | -1 |
| G: -5313.11806 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.33159 HOMO: -7.51851 LUMO: -1.05852 factor:1 | -1 (0.15217) | -1 | -1 |
| G: -5313.11806 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.22342 HOMO: -7.07224 LUMO: -1.89391 factor:1 | -1 (0.26033) | -1 | -1 |
| G: -5313.11806 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.13433 HOMO: -6.65863 LUMO: -0.46804 factor:1 | -1 (0.34942) | -1 | -1 |
| G: -5313.11806 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.29834 HOMO: -7.24367 LUMO: 0.29388 factor:1 | -1 (0.18542) | 1 | 1 |
| G: -5313.11806 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.22571 HOMO: -7.02326 LUMO: -0.87893 factor:1 | -1 (0.25805) | -1 | -1 |
| G: -5313.11806 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.12233 HOMO: -6.88176 LUMO: 0.71566 factor:1 | -1 (0.36142) | -1 | -1 |
| G: -5313.11806 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.17338 HOMO: -6.46543 LUMO: 1.01498 factor:1 | -1 (0.31037) | -1 | -1 |
| G: -5313.11806 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.99752 HOMO: -6.30760 LUMO: 0.17687 factor:1 | -1 (0.48624) | -1 | -1 |
| G: -5313.11806 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.02682 HOMO: -6.73210 LUMO: -1.06941 factor:1 | -1 (0.45693) | -1 | -1 |
| G: -5313.11806 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.08987 HOMO: -6.83550 LUMO: -0.75920 factor:1 | -1 (0.39388) | -1 | -1 |
| G: -5313.11806 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.17028 HOMO: -6.94707 LUMO: 0.42178 factor:1 | -1 (0.31348) | -1 | -1 |
| G: -5313.11806 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.28193 HOMO: -6.77019 LUMO: -0.38096 factor:1 | -1 (0.20183) | -1 | -1 |
| G: -5313.11806 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.68126 HOMO: -7.34163 LUMO: 0.35103 factor:1 | 1 (-0.19750) | 1 | 1 |
| G: -5313.11806 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.87073 HOMO: -6.87632 LUMO: -0.87349 factor:1 | 1 (-0.38697) | -1 | -1 |
| G: -5313.11806 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.64139 HOMO: -7.06952 LUMO: -1.47214 factor:1 | 1 (-0.15764) | -1 | -1 |
| G: -5313.11806 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.89272 HOMO: -6.58788 LUMO: -0.37824 factor:1 | 1 (-0.40896) | -1 | -1 |
| G: -5313.11806 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.62999 HOMO: -6.92802 LUMO: -1.24900 factor:1 | 1 (-0.14623) | -1 | -1 |
| G: -5313.11806 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.95459 HOMO: -7.01237 LUMO: -1.31975 factor:1 | 1 (-0.47084) | -1 | -1 |
| G: -5313.11806 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.05490 HOMO: -6.74842 LUMO: 0.45987 factor:1 | -1 (0.42885) | -1 | -1 |
| G: -5313.11806 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.99806 HOMO: -6.53890 LUMO: 0.94424 factor:1 | -1 (0.48570) | -1 | -1 |
| G: -5313.11806 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.06497 HOMO: -6.52257 LUMO: -0.66940 factor:1 | -1 (0.41878) | -1 | -1 |
| G: -5313.11806 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.12217 HOMO: -6.56883 LUMO: -1.48302 factor:1 | -1 (0.36158) | -1 | -1 |
| G: -5313.11806 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.08105 HOMO: -7.21646 LUMO: 0.13061 factor:1 | -1 (0.40270) | 1 | 1 |
| G: -5313.11806 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.15738 HOMO: -6.62597 LUMO: -0.64763 factor:1 | -1 (0.32637) | -1 | -1 |
| G: -5313.11806 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.20478 HOMO: -7.38789 LUMO: 0.31021 factor:1 | -1 (0.27897) | 1 | 1 |
| G: -5313.11806 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.15923 HOMO: -6.74570 LUMO: -0.70750 factor:1 | -1 (0.32452) | -1 | -1 |
| G: -5313.11806 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.50906 HOMO: -6.95251 LUMO: -1.25989 factor:1 | 1 (-0.02531) | -1 | -1 |
| G: -5313.11806 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.31507 HOMO: -7.13483 LUMO: -0.76736 factor:1 | -1 (0.16868) | -1 | -1 |
| G: -5313.11806 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.22440 HOMO: -6.93618 LUMO: -1.24628 factor:1 | -1 (0.25935) | -1 | -1 |
| G: -5313.11806 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.26255 HOMO: -7.03686 LUMO: 0.26395 factor:1 | -1 (0.22120) | -1 | -1 |
| G: -5313.11806 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.25654 HOMO: -6.52257 LUMO: -0.84355 factor:1 | -1 (0.22722) | -1 | -1 |
| G: -5313.11806 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.12729 HOMO: -6.83278 LUMO: -0.49525 factor:1 | -1 (0.35647) | -1 | -1 |
| G: -5313.11806 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.22789 HOMO: -7.18381 LUMO: -1.64629 factor:1 | -1 (0.25587) | -1 | -1 |
| G: -5313.11806 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.18367 HOMO: -6.74842 LUMO: -0.81090 factor:1 | -1 (0.30009) | -1 | -1 |
| G: -5313.11806 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.06089 HOMO: -7.09401 LUMO: -0.92519 factor:1 | -1 (0.42286) | -1 | -1 |
| G: -5313.11806 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.70915 HOMO: -7.20285 LUMO: -0.81634 factor:1 | 1 (-0.22539) | -1 | -1 |
| G: -5313.11806 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.97250 HOMO: -6.72665 LUMO: 0.77008 factor:1 | 1 (-0.48874) | -1 | -1 |
| G: -5313.11806 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.98733 HOMO: -6.80829 LUMO: 0.86532 factor:1 | 1 (-0.50357) | -1 | -1 |
| G: -5313.11806 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.89506 HOMO: -6.20964 LUMO: 0.99866 factor:1 | 1 (-0.41130) | -1 | -1 |
| G: -5313.11806 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11578.00728 HOMO: -6.52801 LUMO: 1.07757 factor:1 | 1 (-0.52352) | -1 | -1 |
| G: -5313.11806 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.81571 HOMO: -6.74298 LUMO: -0.67756 factor:1 | 1 (-0.33195) | -1 | -1 |
| G: -5313.11806 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.80836 HOMO: -7.43959 LUMO: 0.03265 factor:1 | 1 (-0.32460) | 1 | 1 |
| G: -5313.11806 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.17161 HOMO: -6.46815 LUMO: -0.29933 factor:1 | -1 (0.31214) | -1 | -1 |
| G: -5313.11806 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.31047 HOMO: -6.70489 LUMO: -0.97145 factor:1 | -1 (0.17328) | -1 | -1 |
| G: -5313.11806 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.22168 HOMO: -6.30216 LUMO: -1.39322 factor:1 | -1 (0.26207) | -1 | -1 |
| G: -5313.11806 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.13526 HOMO: -7.01782 LUMO: -1.07485 factor:1 | -1 (0.34850) | -1 | -1 |
| G: -5313.11806 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.58749 HOMO: -6.93074 LUMO: 0.25851 factor:1 | 1 (-0.10373) | -1 | -1 |
| G: -5313.11806 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.71002 HOMO: -7.07224 LUMO: 0.09524 factor:1 | 1 (-0.22626) | 1 | 1 |
| G: -5313.11806 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.74716 HOMO: -6.62325 LUMO: -0.45443 factor:1 | 1 (-0.26341) | -1 | -1 |
| G: -5313.11806 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.88082 HOMO: -7.09945 LUMO: -1.20274 factor:1 | 1 (-0.39707) | -1 | -1 |
| G: -5313.11806 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.70433 HOMO: -6.56067 LUMO: -1.39322 factor:1 | 1 (-0.22058) | -1 | -1 |
| G: -5313.11806 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.57698 HOMO: -6.75387 LUMO: -0.72654 factor:1 | 1 (-0.09323) | -1 | -1 |
| G: -5313.11806 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.69598 HOMO: -6.28583 LUMO: -2.35651 factor:1 | 1 (-0.21222) | -1 | -1 |
| G: -5313.11806 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.75065 HOMO: -6.55522 LUMO: -1.33608 factor:1 | 1 (-0.26689) | -1 | -1 |
| G: -5313.11806 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.51976 HOMO: -7.19741 LUMO: -0.93607 factor:1 | 1 (-0.03600) | -1 | -1 |
| G: -5313.11806 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.58476 HOMO: -6.39740 LUMO: -1.14832 factor:1 | 1 (-0.10101) | -1 | -1 |
| G: -5313.11806 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.88763 HOMO: -7.11850 LUMO: -0.97417 factor:1 | 1 (-0.40387) | -1 | -1 |
| G: -5313.11806 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.91780 HOMO: -6.57699 LUMO: -1.14016 factor:1 | 1 (-0.43405) | -1 | -1 |
| G: -5313.11806 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.67233 HOMO: -6.57699 LUMO: -1.31975 factor:1 | 1 (-0.18857) | -1 | -1 |
| G: -5313.11806 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.71426 HOMO: -6.69128 LUMO: -0.76736 factor:1 | 1 (-0.23051) | -1 | -1 |
| G: -5313.11806 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11578.38712 HOMO: -7.25728 LUMO: 0.29660 factor:1 | 1 (-0.90336) | 1 | 1 |
| G: -5313.11806 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11579.11660 HOMO: -6.37019 LUMO: -0.95240 factor:1 | 1 (-1.63285) | -1 | -1 |
| G: -5313.11806 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11578.42862 HOMO: -6.48447 LUMO: -0.55511 factor:1 | 1 (-0.94486) | -1 | -1 |
| G: -5313.11806 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.91500 HOMO: -6.37291 LUMO: -0.78641 factor:1 | 1 (-0.43125) | -1 | -1 |
| G: -5313.11806 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.91029 HOMO: -6.65863 LUMO: -0.69933 factor:1 | 1 (-0.42654) | -1 | -1 |
| G: -5313.11806 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11578.02831 HOMO: -6.44638 LUMO: -0.16055 factor:1 | 1 (-0.54455) | -1 | -1 |
| G: -5313.11806 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11578.37950 HOMO: -6.41917 LUMO: -0.20136 factor:1 | 1 (-0.89574) | -1 | -1 |
| G: -5313.11806 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11578.22298 HOMO: -7.33347 LUMO: 0.12789 factor:1 | 1 (-0.73922) | 1 | 1 |
| G: -5313.11806 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11578.33262 HOMO: -6.70489 LUMO: -0.52518 factor:1 | 1 (-0.84886) | -1 | -1 |
| G: -5313.11806 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.01199 HOMO: -7.25183 LUMO: 0.32109 factor:1 | -1 (0.47176) | 1 | 1 |
| G: -5313.11806 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.90432 HOMO: -7.29265 LUMO: 0.28028 factor:1 | -1 (0.57944) | 1 | 1 |
| G: -5313.11806 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.92502 HOMO: -6.57155 LUMO: -0.51702 factor:1 | -1 (0.55873) | -1 | -1 |
| G: -5313.11806 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.15861 HOMO: -7.08040 LUMO: 0.39729 factor:1 | -1 (0.32515) | 1 | 1 |
| G: -5313.11806 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11578.59148 HOMO: -6.24501 LUMO: -0.44627 factor:1 | 1 (-1.10772) | -1 | -1 |
| G: -5313.11806 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.94219 HOMO: -6.73754 LUMO: -0.45443 factor:1 | 1 (-0.45843) | -1 | -1 |
| G: -5313.11806 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.91201 HOMO: -6.24501 LUMO: 0.38096 factor:1 | 1 (-0.42825) | -1 | -1 |
| G: -5313.11806 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.96205 HOMO: -6.86815 LUMO: -0.91974 factor:1 | 1 (-0.47829) | -1 | -1 |
| G: -5313.11806 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.99577 HOMO: -7.40150 LUMO: 0.36191 factor:1 | -1 (0.48798) | 1 | 1 |
| G: -5313.11806 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.90045 HOMO: -6.44094 LUMO: -0.64219 factor:1 | -1 (0.58330) | -1 | -1 |
| G: -5313.11806 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.05071 HOMO: -6.69944 LUMO: -0.80001 factor:1 | -1 (0.43304) | -1 | -1 |
| G: -5313.11806 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.38057 HOMO: -6.61509 LUMO: -0.70750 factor:1 | -1 (0.10319) | -1 | -1 |
| G: -5313.11806 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.16176 HOMO: -7.52123 LUMO: 0.06803 factor:1 | -1 (0.32199) | 1 | 1 |
| G: -5313.11806 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.94481 HOMO: -7.34163 LUMO: 0.30477 factor:1 | -1 (0.53895) | 1 | 1 |
| G: -5313.11806 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.86679 HOMO: -6.68584 LUMO: -0.78641 factor:1 | -1 (0.61696) | -1 | -1 |
| G: -5313.11806 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.16906 HOMO: -6.53890 LUMO: -0.50885 factor:1 | -1 (0.31470) | -1 | -1 |
| G: -5313.11806 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.93460 HOMO: -6.75659 LUMO: -0.68845 factor:1 | -1 (0.54915) | -1 | -1 |
| G: -5313.11806 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.21706 HOMO: -7.08857 LUMO: 0.43266 factor:1 | -1 (0.26670) | 1 | 1 |
| G: -5313.11806 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.88181 HOMO: -6.28583 LUMO: -0.46804 factor:1 | -1 (0.60194) | -1 | -1 |
| G: -5313.11806 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.90274 HOMO: -6.50080 LUMO: -0.24762 factor:1 | -1 (0.58102) | -1 | -1 |
| G: -5313.11806 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.03129 HOMO: -6.45454 LUMO: -0.58504 factor:1 | -1 (0.45247) | -1 | -1 |
| G: -5313.11806 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.05471 HOMO: -7.20558 LUMO: 0.20953 factor:1 | -1 (0.42904) | 1 | 1 |
| G: -5313.11806 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.27061 HOMO: -6.35930 LUMO: -0.20681 factor:1 | -1 (0.21315) | -1 | -1 |
| G: -5313.11806 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.14631 HOMO: -6.36202 LUMO: -0.14422 factor:1 | -1 (0.33745) | -1 | -1 |
| G: -5313.11806 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.00557 HOMO: -6.20692 LUMO: 1.97827 factor:1 | -1 (0.47819) | -1 | -1 |
| G: -5313.11806 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.11578 HOMO: -6.48719 LUMO: 1.74153 factor:1 | -1 (0.36798) | -1 | -1 |
| G: -5313.11806 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.31690 HOMO: -6.84638 LUMO: 1.88575 factor:1 | -1 (0.16686) | -1 | -1 |
| G: -5313.11806 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.00252 HOMO: -5.90759 LUMO: 2.00820 factor:1 | -1 (0.48123) | -1 | -1 |
| G: -5313.11806 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.12522 HOMO: -6.56339 LUMO: 1.99732 factor:1 | -1 (0.35854) | -1 | -1 |
| G: -5313.11806 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.01020 HOMO: -6.20692 LUMO: 1.75241 factor:1 | -1 (0.47356) | -1 | -1 |
| G: -5313.11806 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.08067 HOMO: -6.16882 LUMO: 1.94017 factor:1 | -1 (0.40308) | -1 | -1 |
| G: -5313.11806 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.06127 HOMO: -6.80829 LUMO: 1.78507 factor:1 | -1 (0.42248) | -1 | -1 |
| G: -5313.11806 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.15706 HOMO: -6.58243 LUMO: 1.78235 factor:1 | -1 (0.32670) | -1 | -1 |
| G: -5313.11806 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.65244 HOMO: -5.85045 LUMO: 1.82316 factor:1 | 1 (-0.16868) | -1 | -1 |
| G: -5313.11806 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.76240 HOMO: -5.93752 LUMO: 1.56465 factor:1 | 1 (-0.27864) | -1 | -1 |
| G: -5313.11806 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.95296 HOMO: -6.59604 LUMO: -0.53334 factor:1 | 1 (-0.46921) | -1 | -1 |
| G: -5313.11806 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.53309 HOMO: -7.06135 LUMO: 0.29660 factor:1 | 1 (-0.04933) | 1 | 1 |
| G: -5313.11806 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.78809 HOMO: -6.50352 LUMO: 1.61908 factor:1 | 1 (-0.30433) | -1 | -1 |
| G: -5313.11806 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.64134 HOMO: -6.68040 LUMO: -0.60681 factor:1 | 1 (-0.15758) | -1 | -1 |
| G: -5313.11806 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11578.02616 HOMO: -6.93618 LUMO: -1.09662 factor:1 | 1 (-0.54240) | -1 | -1 |
| G: -5313.11806 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.81554 HOMO: -6.72121 LUMO: -1.14016 factor:1 | 1 (-0.33179) | -1 | -1 |
| G: -5313.11806 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.89647 HOMO: -7.12394 LUMO: -1.24900 factor:1 | 1 (-0.41272) | -1 | -1 |
| G: -5313.11806 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.96118 HOMO: -6.71305 LUMO: -0.71566 factor:1 | 1 (-0.47742) | -1 | -1 |
| G: -5313.11806 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.97621 HOMO: -7.09401 LUMO: -0.86532 factor:1 | -1 (0.50755) | -1 | -1 |
| G: -5313.11806 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.02353 HOMO: -7.08584 LUMO: -0.92519 factor:1 | -1 (0.46023) | -1 | -1 |
| G: -5313.11806 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.14419 HOMO: -7.05591 LUMO: 0.11973 factor:1 | -1 (0.33957) | -1 | -1 |
| G: -5313.11806 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.08429 HOMO: -7.14843 LUMO: -1.58370 factor:1 | -1 (0.39946) | -1 | -1 |
| G: -5313.11806 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.99433 HOMO: -7.36884 LUMO: -1.97010 factor:1 | -1 (0.48942) | -1 | -1 |
| G: -5313.11806 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.78886 HOMO: -6.81373 LUMO: -1.72248 factor:1 | -1 (0.69490) | -1 | -1 |
| G: -5313.11806 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.83689 HOMO: -6.87360 LUMO: -1.03947 factor:1 | -1 (0.64687) | -1 | -1 |
| G: -5313.11806 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.91945 HOMO: -7.02870 LUMO: -0.87349 factor:1 | -1 (0.56431) | -1 | -1 |
| G: -5313.11806 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.97485 HOMO: -7.16476 LUMO: -1.18097 factor:1 | -1 (0.50891) | -1 | -1 |
| G: -5313.11806 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.14516 HOMO: -7.51851 LUMO: 0.07891 factor:1 | -1 (0.33859) | 1 | 1 |
| G: -5313.11806 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.85101 HOMO: -7.04231 LUMO: -0.83539 factor:1 | -1 (0.63275) | -1 | -1 |
| G: -5313.11806 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.75041 HOMO: -6.83278 LUMO: -0.60137 factor:1 | -1 (0.73335) | -1 | -1 |
| G: -5313.11806 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.88045 HOMO: -6.89809 LUMO: -1.19186 factor:1 | -1 (0.60330) | -1 | -1 |
| G: -5313.11806 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.78189 HOMO: -7.16476 LUMO: -0.79185 factor:1 | -1 (0.70186) | -1 | -1 |
| G: -5313.11806 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.06329 HOMO: -6.97156 LUMO: -1.25444 factor:1 | -1 (0.42047) | -1 | -1 |
| G: -5313.11806 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.90037 HOMO: -6.84366 LUMO: -0.88437 factor:1 | -1 (0.58338) | -1 | -1 |
| G: -5313.11806 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.05787 HOMO: -6.91986 LUMO: -1.12655 factor:1 | -1 (0.42589) | -1 | -1 |
| G: -5313.11806 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11578.95440 HOMO: -6.49536 LUMO: -0.29660 factor:1 | 1 (-1.47064) | -1 | -1 |
| G: -5313.11806 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11578.00401 HOMO: -6.74842 LUMO: 0.42450 factor:1 | 1 (-0.52025) | -1 | -1 |
| G: -5313.11806 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11578.22633 HOMO: -7.34435 LUMO: 0.32109 factor:1 | 1 (-0.74257) | 1 | 1 |
| G: -5313.11806 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11578.35074 HOMO: -7.16476 LUMO: 0.28572 factor:1 | 1 (-0.86698) | 1 | 1 |
| G: -5313.11806 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.72037 HOMO: -6.74298 LUMO: -0.43538 factor:1 | -1 (0.76339) | -1 | -1 |
| G: -5313.11806 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.85237 HOMO: -7.19469 LUMO: -1.61091 factor:1 | -1 (0.63139) | -1 | -1 |
| G: -5313.11806 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.97158 HOMO: -7.35252 LUMO: -1.78235 factor:1 | -1 (0.51217) | -1 | -1 |
| G: -5313.11806 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.81248 HOMO: -7.25456 LUMO: -1.66806 factor:1 | -1 (0.67128) | -1 | -1 |
| G: -5313.11806 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.69759 HOMO: -7.54844 LUMO: -1.07213 factor:1 | -1 (0.78616) | -1 | -1 |
| G: -5313.11806 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11578.44543 HOMO: -7.21918 LUMO: -1.55377 factor:1 | 1 (-0.96168) | -1 | -1 |
| G: -5313.11806 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.65519 HOMO: -7.01782 LUMO: -1.60547 factor:1 | 1 (-0.17143) | -1 | -1 |
| G: -5313.11806 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.75337 HOMO: -7.21646 LUMO: -1.53472 factor:1 | 1 (-0.26961) | -1 | -1 |
| G: -5313.11806 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.83933 HOMO: -6.73754 LUMO: -1.37417 factor:1 | 1 (-0.35557) | -1 | -1 |
| G: -5313.11806 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.96779 HOMO: -6.78924 LUMO: 0.66396 factor:1 | 1 (-0.48404) | -1 | -1 |
| G: -5313.11806 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.95855 HOMO: -6.82734 LUMO: 0.61226 factor:1 | -1 (0.52521) | -1 | -1 |
| G: -5313.11806 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.21649 HOMO: -6.74026 LUMO: 0.65579 factor:1 | -1 (0.26727) | -1 | -1 |
| G: -5313.11806 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.91822 HOMO: -7.10489 LUMO: -1.30887 factor:1 | -1 (0.56553) | -1 | -1 |
| G: -5313.11806 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.98994 HOMO: -7.05047 LUMO: 0.42722 factor:1 | 1 (-0.50619) | -1 | -1 |
| G: -5313.11806 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.99277 HOMO: -6.61237 LUMO: 1.30887 factor:1 | 1 (-0.50902) | -1 | -1 |
| G: -5313.11806 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.87527 HOMO: -7.05863 LUMO: 0.59049 factor:1 | 1 (-0.39152) | -1 | -1 |
| G: -5313.11806 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.86178 HOMO: -6.26406 LUMO: 0.78641 factor:1 | 1 (-0.37802) | -1 | -1 |
| G: -5313.11806 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.93106 HOMO: -6.70489 LUMO: 0.67756 factor:1 | 1 (-0.44730) | -1 | -1 |
| G: -5313.11806 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11578.52731 HOMO: -6.78652 LUMO: -0.94968 factor:1 | 1 (-1.04356) | -1 | -1 |
| G: -5313.11806 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.20008 HOMO: -6.36202 LUMO: -0.94424 factor:1 | -1 (0.28368) | -1 | -1 |
| G: -5313.11806 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11578.21245 HOMO: -6.81645 LUMO: -1.09934 factor:1 | 1 (-0.72869) | -1 | -1 |
| G: -5313.11806 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11578.08701 HOMO: -7.07224 LUMO: 0.85988 factor:1 | 1 (-0.60325) | 1 | 1 |
| G: -5313.11806 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.99424 HOMO: -7.02326 LUMO: 1.10206 factor:1 | 1 (-0.51049) | -1 | -1 |
| G: -5313.11806 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.67342 HOMO: -6.71305 LUMO: 0.84627 factor:1 | 1 (-0.18966) | -1 | -1 |
| G: -5313.11806 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.91821 HOMO: -7.27360 LUMO: 0.88165 factor:1 | 1 (-0.43446) | 1 | 1 |
| G: -5313.11806 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11578.06709 HOMO: -6.84911 LUMO: 0.59865 factor:1 | 1 (-0.58333) | -1 | -1 |
| G: -5313.11806 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.82091 HOMO: -6.75114 LUMO: -2.49801 factor:1 | 1 (-0.33715) | -1 | -1 |
| G: -5313.11806 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.66515 HOMO: -6.97156 LUMO: 0.53606 factor:1 | 1 (-0.18139) | -1 | -1 |
| G: -5313.11806 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.37486 HOMO: -6.54434 LUMO: 0.73199 factor:1 | -1 (0.10890) | -1 | -1 |
| G: -5313.11806 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.47339 HOMO: -6.21236 LUMO: 0.99866 factor:1 | -1 (0.01037) | -1 | -1 |
| G: -5313.11806 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.45910 HOMO: -6.34025 LUMO: 0.50341 factor:1 | -1 (0.02465) | -1 | -1 |
| G: -5313.11806 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.26756 HOMO: -6.59876 LUMO: -0.69389 factor:1 | -1 (0.21619) | -1 | -1 |
| G: -5313.11806 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.88371 HOMO: -6.54978 LUMO: -1.00682 factor:1 | 1 (-0.39995) | -1 | -1 |
| G: -5313.11806 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.62332 HOMO: -6.82462 LUMO: -0.98777 factor:1 | 1 (-0.13957) | -1 | -1 |
| G: -5313.11806 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.62354 HOMO: -6.85455 LUMO: -0.68573 factor:1 | 1 (-0.13978) | -1 | -1 |
| G: -5313.11806 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.48607 HOMO: -7.55388 LUMO: -0.03265 factor:1 | 1 (-0.00231) | 1 | 1 |
| G: -5313.11806 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.54626 HOMO: -6.77019 LUMO: -0.71838 factor:1 | 1 (-0.06250) | -1 | -1 |
| G: -5313.11806 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.46640 HOMO: -6.84911 LUMO: -1.25444 factor:1 | -1 (0.01736) | -1 | -1 |
| G: -5313.11806 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.40193 HOMO: -6.95251 LUMO: -1.03675 factor:1 | -1 (0.08182) | -1 | -1 |
| G: -5313.11806 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.17673 HOMO: -6.80829 LUMO: -0.77280 factor:1 | -1 (0.30703) | -1 | -1 |
| G: -5313.11806 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.32386 HOMO: -6.94162 LUMO: -0.94151 factor:1 | -1 (0.15989) | -1 | -1 |
| G: -5313.11806 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.29080 HOMO: -6.89809 LUMO: -0.90886 factor:1 | -1 (0.19296) | -1 | -1 |
| G: -5313.11806 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.73803 HOMO: -6.85183 LUMO: -0.88981 factor:1 | -1 (0.74573) | -1 | -1 |
| G: -5313.11806 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.10696 HOMO: -6.51985 LUMO: -0.84627 factor:1 | -1 (0.37680) | -1 | -1 |
| G: -5313.11806 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.27080 HOMO: -6.83278 LUMO: -1.08029 factor:1 | -1 (0.21296) | -1 | -1 |
| G: -5313.11806 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.31456 HOMO: -6.91986 LUMO: 0.66396 factor:1 | -1 (0.16920) | -1 | -1 |
| G: -5313.11806 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.44906 HOMO: -6.94162 LUMO: 0.50885 factor:1 | -1 (0.03469) | -1 | -1 |
| G: -5313.11806 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.46435 HOMO: -6.94435 LUMO: 0.80546 factor:1 | -1 (0.01940) | -1 | -1 |
| G: -5313.11806 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.85116 HOMO: -6.74298 LUMO: -0.81634 factor:1 | 1 (-0.36741) | -1 | -1 |
| G: -5313.11806 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11578.06088 HOMO: -7.04503 LUMO: 1.15921 factor:1 | 1 (-0.57713) | -1 | -1 |
| G: -5313.11806 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11578.02202 HOMO: -6.76475 LUMO: 0.75920 factor:1 | 1 (-0.53827) | -1 | -1 |
| G: -5313.11806 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11578.21381 HOMO: -7.05047 LUMO: 0.68845 factor:1 | 1 (-0.73005) | -1 | -1 |
| G: -5313.11806 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.77380 HOMO: -7.12666 LUMO: 0.60681 factor:1 | 1 (-0.29005) | 1 | 1 |
| G: -5313.11806 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11578.00850 HOMO: -6.90897 LUMO: -1.22723 factor:1 | 1 (-0.52474) | -1 | -1 |
| G: -5313.11806 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.95089 HOMO: -7.10761 LUMO: 0.58232 factor:1 | 1 (-0.46714) | 1 | 1 |
| G: -5313.11806 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11578.06075 HOMO: -6.57427 LUMO: 0.71294 factor:1 | 1 (-0.57699) | -1 | -1 |
| G: -5313.11806 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.89399 HOMO: -6.22597 LUMO: 0.99322 factor:1 | 1 (-0.41024) | -1 | -1 |
| G: -5313.11806 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11578.14146 HOMO: -6.83550 LUMO: -0.77825 factor:1 | 1 (-0.65770) | -1 | -1 |
| G: -5313.11806 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.70452 HOMO: -7.14843 LUMO: 0.44627 factor:1 | 1 (-0.22077) | 1 | 1 |
| G: -5313.11806 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.86997 HOMO: -7.08040 LUMO: 0.78913 factor:1 | 1 (-0.38621) | 1 | 1 |
| G: -5313.11806 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.77571 HOMO: -6.81373 LUMO: -0.93879 factor:1 | 1 (-0.29195) | -1 | -1 |
| G: -5313.11806 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.81361 HOMO: -6.95251 LUMO: 0.22585 factor:1 | 1 (-0.32986) | -1 | -1 |
| G: -5313.11806 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.86338 HOMO: -7.13483 LUMO: -1.25444 factor:1 | 1 (-0.37963) | -1 | -1 |
| G: -5313.11806 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11578.22701 HOMO: -6.37835 LUMO: -1.54289 factor:1 | 1 (-0.74325) | -1 | -1 |
| G: -5313.11806 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11578.04143 HOMO: -6.53617 LUMO: -1.43948 factor:1 | 1 (-0.55767) | -1 | -1 |
| G: -5313.11806 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11578.00494 HOMO: -6.38379 LUMO: 0.16055 factor:1 | 1 (-0.52118) | -1 | -1 |
| G: -5313.11806 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.23273 HOMO: -6.53617 LUMO: 0.15783 factor:1 | -1 (0.25103) | -1 | -1 |
| G: -5313.11806 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.31940 HOMO: -6.79740 LUMO: -0.17960 factor:1 | -1 (0.16436) | -1 | -1 |
| G: -5313.11806 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.90151 HOMO: -6.26678 LUMO: -0.41361 factor:1 | -1 (0.58224) | -1 | -1 |
| G: -5313.11806 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.00786 HOMO: -6.35658 LUMO: -0.24218 factor:1 | -1 (0.47590) | -1 | -1 |
| G: -5313.11806 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.24511 HOMO: -6.48175 LUMO: -0.71566 factor:1 | -1 (0.23864) | -1 | -1 |
| G: -5313.11806 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.43682 HOMO: -6.21508 LUMO: -0.40001 factor:1 | -1 (0.04694) | -1 | -1 |
| G: -5313.11806 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.83966 HOMO: -6.51985 LUMO: -0.32654 factor:1 | -1 (0.64409) | -1 | -1 |
| G: -5313.11806 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.07820 HOMO: -6.45182 LUMO: -0.66396 factor:1 | -1 (0.40556) | -1 | -1 |
| G: -5313.11806 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.27589 HOMO: -6.51441 LUMO: -0.65307 factor:1 | -1 (0.20787) | -1 | -1 |
| G: -5313.11806 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.84099 HOMO: -6.57971 LUMO: -0.92519 factor:1 | 1 (-0.35723) | -1 | -1 |
| G: -5313.11806 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.84602 HOMO: -6.67223 LUMO: -0.58232 factor:1 | 1 (-0.36227) | -1 | -1 |
| G: -5313.11806 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.77715 HOMO: -6.10351 LUMO: -0.45987 factor:1 | 1 (-0.29339) | -1 | -1 |
| G: -5313.11806 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.77601 HOMO: -6.13889 LUMO: -0.50341 factor:1 | 1 (-0.29225) | -1 | -1 |
| G: -5313.11806 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.84099 HOMO: -6.63141 LUMO: -0.28300 factor:1 | 1 (-0.35723) | -1 | -1 |
| G: -5313.11806 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.76071 HOMO: -6.37563 LUMO: -0.22858 factor:1 | 1 (-0.27696) | -1 | -1 |
| G: -5313.11806 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.82929 HOMO: -6.37019 LUMO: 0.11429 factor:1 | 1 (-0.34553) | -1 | -1 |
| G: -5313.11806 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.83998 HOMO: -6.23957 LUMO: 0.28844 factor:1 | 1 (-0.35622) | -1 | -1 |
| G: -5313.11806 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11578.06382 HOMO: -6.41372 LUMO: -0.53879 factor:1 | 1 (-0.58007) | -1 | -1 |
| G: -5313.11806 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11578.05656 HOMO: -7.06680 LUMO: 0.32654 factor:1 | 1 (-0.57280) | 1 | 1 |
| G: -5313.11806 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.78877 HOMO: -6.50896 LUMO: -0.73743 factor:1 | 1 (-0.30501) | -1 | -1 |
| G: -5313.11806 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.94172 HOMO: -6.42189 LUMO: -0.28572 factor:1 | 1 (-0.45797) | -1 | -1 |
| G: -5313.11806 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.96847 HOMO: -6.79740 LUMO: -0.25851 factor:1 | 1 (-0.48472) | -1 | -1 |
| G: -5313.11806 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.95070 HOMO: -6.32393 LUMO: 0.17960 factor:1 | 1 (-0.46695) | -1 | -1 |
| G: -5313.11806 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.86142 HOMO: -6.65046 LUMO: 0.03537 factor:1 | 1 (-0.37767) | -1 | -1 |
| G: -5313.11806 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.97636 HOMO: -6.60148 LUMO: 0.07619 factor:1 | 1 (-0.49261) | -1 | -1 |
| G: -5313.11806 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.71573 HOMO: -6.57971 LUMO: 0.11429 factor:1 | 1 (-0.23198) | -1 | -1 |
| G: -5313.11806 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11578.05544 HOMO: -6.88448 LUMO: -1.21907 factor:1 | 1 (-0.57168) | -1 | -1 |
| G: -5313.11806 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11578.06317 HOMO: -6.97700 LUMO: 0.36463 factor:1 | 1 (-0.57941) | -1 | -1 |
| G: -5313.11806 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11578.09218 HOMO: -6.73210 LUMO: -0.84083 factor:1 | 1 (-0.60842) | -1 | -1 |
| G: -5313.11806 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.77130 HOMO: -6.21236 LUMO: -0.68845 factor:1 | 1 (-0.28754) | -1 | -1 |
| G: -5313.11806 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.76115 HOMO: -6.35658 LUMO: -0.82995 factor:1 | 1 (-0.27739) | -1 | -1 |
| G: -5313.11806 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11578.03054 HOMO: -6.75114 LUMO: -0.94424 factor:1 | 1 (-0.54679) | -1 | -1 |
| G: -5313.11806 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.76855 HOMO: -6.74026 LUMO: -1.46125 factor:1 | 1 (-0.28479) | -1 | -1 |
| G: -5313.11806 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.89979 HOMO: -7.06952 LUMO: 0.91974 factor:1 | 1 (-0.41603) | 1 | 1 |
| G: -5313.11806 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.75244 HOMO: -7.08857 LUMO: 0.74559 factor:1 | 1 (-0.26869) | 1 | 1 |
| G: -5313.11806 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.68357 HOMO: -6.74298 LUMO: 1.03131 factor:1 | 1 (-0.19981) | -1 | -1 |
| G: -5313.11806 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.96059 HOMO: -6.74842 LUMO: -1.77962 factor:1 | -1 (0.52317) | -1 | -1 |
| G: -5313.11806 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.28223 HOMO: -6.82462 LUMO: -1.61908 factor:1 | -1 (0.20153) | -1 | -1 |
| G: -5313.11806 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.07545 HOMO: -7.17020 LUMO: -1.02043 factor:1 | -1 (0.40831) | -1 | -1 |
| G: -5313.11806 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.03052 HOMO: -6.26406 LUMO: -0.96328 factor:1 | -1 (0.45323) | -1 | -1 |
| G: -5313.11806 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.86180 HOMO: -6.50896 LUMO: -0.38640 factor:1 | 1 (-0.37805) | -1 | -1 |
| G: -5313.11806 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.72137 HOMO: -7.27632 LUMO: -1.17553 factor:1 | 1 (-0.23761) | -1 | -1 |
| G: -5313.11806 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11578.10442 HOMO: -6.54162 LUMO: -1.36873 factor:1 | 1 (-0.62066) | -1 | -1 |
| G: -5313.11806 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.94834 HOMO: -6.42733 LUMO: -1.15648 factor:1 | 1 (-0.46458) | -1 | -1 |
| G: -5313.11806 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.93908 HOMO: -6.73754 LUMO: -2.58780 factor:1 | 1 (-0.45533) | -1 | -1 |
| G: -5313.11806 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11578.05239 HOMO: -7.20285 LUMO: 0.75103 factor:1 | 1 (-0.56864) | 1 | 1 |
| G: -5313.11806 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.78537 HOMO: -6.98788 LUMO: 0.34831 factor:1 | 1 (-0.30161) | -1 | -1 |
| G: -5313.11806 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.85157 HOMO: -6.80013 LUMO: -1.11567 factor:1 | 1 (-0.36782) | -1 | -1 |
| G: -5313.11806 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11578.03854 HOMO: -6.67767 LUMO: -0.82450 factor:1 | 1 (-0.55479) | -1 | -1 |
| G: -5313.11806 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11578.06763 HOMO: -6.84911 LUMO: -0.21497 factor:1 | 1 (-0.58387) | -1 | -1 |
| G: -5313.11806 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11578.09294 HOMO: -6.23141 LUMO: 0.21769 factor:1 | 1 (-0.60918) | -1 | -1 |
| G: -5313.11806 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.93631 HOMO: -6.68312 LUMO: 0.16327 factor:1 | 1 (-0.45255) | -1 | -1 |
| G: -5313.11806 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.77212 HOMO: -7.04503 LUMO: -1.04220 factor:1 | 1 (-0.28836) | -1 | -1 |
| G: -5313.11806 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.61630 HOMO: -6.67495 LUMO: -0.71294 factor:1 | 1 (-0.13255) | -1 | -1 |
| G: -5313.11806 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.80455 HOMO: -6.70216 LUMO: -0.55239 factor:1 | 1 (-0.32080) | -1 | -1 |
| G: -5313.11806 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.87865 HOMO: -6.60420 LUMO: -0.71294 factor:1 | 1 (-0.39489) | -1 | -1 |
| G: -5313.11806 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.74014 HOMO: -7.40694 LUMO: 0.11973 factor:1 | 1 (-0.25639) | 1 | 1 |
| G: -5313.11806 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.56972 HOMO: -6.58788 LUMO: -0.29116 factor:1 | 1 (-0.08596) | -1 | -1 |
| G: -5313.11806 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.44552 HOMO: -6.63686 LUMO: -0.32654 factor:1 | -1 (0.03823) | -1 | -1 |
| G: -5313.11806 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.59935 HOMO: -6.85183 LUMO: -0.95512 factor:1 | 1 (-0.11559) | -1 | -1 |
| G: -5313.11806 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.52329 HOMO: -6.82189 LUMO: -0.88165 factor:1 | 1 (-0.03954) | -1 | -1 |
| G: -5313.11806 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.71383 HOMO: -6.97428 LUMO: -1.03947 factor:1 | 1 (-0.23007) | -1 | -1 |
| G: -5313.11806 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.42596 HOMO: -6.51441 LUMO: -0.05714 factor:1 | -1 (0.05780) | -1 | -1 |
| G: -5313.11806 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.65685 HOMO: -6.61509 LUMO: -0.77008 factor:1 | 1 (-0.17309) | -1 | -1 |
| G: -5313.11806 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.50610 HOMO: -7.36340 LUMO: 0.29116 factor:1 | 1 (-0.02234) | 1 | 1 |
| G: -5313.11806 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.60893 HOMO: -6.64230 LUMO: -0.79185 factor:1 | 1 (-0.12517) | -1 | -1 |
| G: -5313.11806 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.82452 HOMO: -6.56883 LUMO: -1.03403 factor:1 | 1 (-0.34077) | -1 | -1 |
| G: -5313.11806 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.53584 HOMO: -6.69400 LUMO: -0.77825 factor:1 | 1 (-0.05208) | -1 | -1 |
| G: -5313.11806 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.48803 HOMO: -6.37019 LUMO: -0.79185 factor:1 | 1 (-0.00427) | -1 | -1 |
| G: -5313.11806 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.43894 HOMO: -6.49808 LUMO: -0.94424 factor:1 | -1 (0.04482) | -1 | -1 |
| G: -5313.11806 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.72343 HOMO: -6.91713 LUMO: -0.75376 factor:1 | 1 (-0.23968) | -1 | -1 |
| G: -5313.11806 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.63081 HOMO: -7.13755 LUMO: 0.41361 factor:1 | 1 (-0.14705) | 1 | 1 |
| G: -5313.11806 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.70928 HOMO: -7.12122 LUMO: 0.39457 factor:1 | 1 (-0.22553) | 1 | 1 |
| G: -5313.11806 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.74349 HOMO: -6.59332 LUMO: -0.57144 factor:1 | 1 (-0.25973) | -1 | -1 |
| G: -5313.11806 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.83481 HOMO: -6.62325 LUMO: -0.66940 factor:1 | 1 (-0.35105) | -1 | -1 |
| G: -5313.11806 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11578.05411 HOMO: -6.90897 LUMO: -0.08708 factor:1 | 1 (-0.57035) | -1 | -1 |
| G: -5313.11806 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.79761 HOMO: -6.65591 LUMO: -0.81090 factor:1 | 1 (-0.31386) | -1 | -1 |
| G: -5313.11806 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.76428 HOMO: -6.65318 LUMO: -0.94696 factor:1 | 1 (-0.28052) | -1 | -1 |
| G: -5313.11806 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.75108 HOMO: -6.96067 LUMO: -1.03675 factor:1 | 1 (-0.26732) | -1 | -1 |
| G: -5313.11806 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.91136 HOMO: -6.23141 LUMO: -0.66396 factor:1 | 1 (-0.42760) | -1 | -1 |
| G: -5313.11806 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.70488 HOMO: -6.52529 LUMO: -0.78369 factor:1 | 1 (-0.22112) | -1 | -1 |
| G: -5313.11806 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.78934 HOMO: -6.39468 LUMO: -0.40817 factor:1 | 1 (-0.30558) | -1 | -1 |
| G: -5313.11806 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.48343 HOMO: -6.76203 LUMO: -0.20409 factor:1 | -1 (0.00033) | -1 | -1 |
| G: -5313.11806 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.43818 HOMO: -6.96611 LUMO: -0.90342 factor:1 | -1 (0.04558) | -1 | -1 |
| G: -5313.11806 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.54229 HOMO: -6.54706 LUMO: -0.87893 factor:1 | 1 (-0.05853) | -1 | -1 |
| G: -5313.11806 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.43543 HOMO: -7.24367 LUMO: -0.97689 factor:1 | -1 (0.04833) | -1 | -1 |
| G: -5313.11806 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.34990 HOMO: -6.61781 LUMO: 1.43404 factor:1 | -1 (0.13385) | -1 | -1 |
| G: -5313.11806 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.39061 HOMO: -6.17971 LUMO: 1.79867 factor:1 | -1 (0.09314) | -1 | -1 |
| G: -5313.11806 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.64136 HOMO: -5.73344 LUMO: 2.13609 factor:1 | 1 (-0.15761) | -1 | -1 |
| G: -5313.11806 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.42732 HOMO: -6.72121 LUMO: 2.06807 factor:1 | -1 (0.05644) | -1 | -1 |
| G: -5313.11806 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.73405 HOMO: -6.91169 LUMO: 2.02997 factor:1 | 1 (-0.25029) | -1 | -1 |
| G: -5313.11806 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.48950 HOMO: -7.06408 LUMO: 1.41499 factor:1 | 1 (-0.00574) | 1 | 1 |
| G: -5313.11806 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.33015 HOMO: -6.94162 LUMO: -0.90070 factor:1 | -1 (0.15361) | -1 | -1 |
| G: -5313.11806 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.27763 HOMO: -7.09401 LUMO: 0.35103 factor:1 | -1 (0.20613) | 1 | 1 |
| G: -5313.11806 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.17774 HOMO: -6.78652 LUMO: 0.91974 factor:1 | -1 (0.30602) | -1 | -1 |
| G: -5313.11806 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.93550 HOMO: -6.32937 LUMO: -1.89119 factor:1 | -1 (0.54826) | -1 | -1 |
| G: -5313.11806 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.42231 HOMO: -7.12666 LUMO: -1.06397 factor:1 | -1 (0.06144) | -1 | -1 |
| G: -5313.11806 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.22381 HOMO: -6.38107 LUMO: -1.43132 factor:1 | -1 (0.25995) | -1 | -1 |
| G: -5313.11806 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.11708 HOMO: -7.09129 LUMO: 0.08980 factor:1 | -1 (0.36667) | 1 | 1 |
| G: -5313.11806 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.60969 HOMO: -6.31304 LUMO: -0.57960 factor:1 | 1 (-0.12593) | -1 | -1 |
| G: -5313.11806 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.16239 HOMO: -6.94435 LUMO: -0.74287 factor:1 | -1 (0.32137) | -1 | -1 |
| G: -5313.11806 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.27962 HOMO: -6.35658 LUMO: -1.53472 factor:1 | -1 (0.20414) | -1 | -1 |
| G: -5313.11806 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.36359 HOMO: -6.39740 LUMO: -1.48846 factor:1 | -1 (0.12017) | -1 | -1 |
| G: -5313.11806 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11578.11743 HOMO: -7.05319 LUMO: -0.33198 factor:1 | 1 (-0.63367) | -1 | -1 |
| G: -5313.11806 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11578.01816 HOMO: -6.68040 LUMO: -0.09252 factor:1 | 1 (-0.53440) | -1 | -1 |
| G: -5313.11806 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11578.34641 HOMO: -6.35930 LUMO: -0.43266 factor:1 | 1 (-0.86266) | -1 | -1 |
| G: -5313.11806 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.81614 HOMO: -6.59604 LUMO: -1.45853 factor:1 | 1 (-0.33239) | -1 | -1 |
| G: -5313.11806 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11578.72579 HOMO: -6.46270 LUMO: -1.49391 factor:1 | 1 (-1.24204) | -1 | -1 |
| G: -5313.11806 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11578.20976 HOMO: -7.05863 LUMO: -1.04764 factor:1 | 1 (-0.72600) | -1 | -1 |
| G: -5313.11806 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11578.40336 HOMO: -7.14027 LUMO: -0.81634 factor:1 | 1 (-0.91961) | -1 | -1 |
| G: -5313.11806 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11578.39887 HOMO: -6.80285 LUMO: -0.74287 factor:1 | 1 (-0.91512) | -1 | -1 |
| G: -5313.11806 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11578.77831 HOMO: -6.53890 LUMO: -1.13471 factor:1 | 1 (-1.29455) | -1 | -1 |
| G: -5313.11806 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11578.21773 HOMO: -6.49808 LUMO: -1.35513 factor:1 | 1 (-0.73397) | -1 | -1 |
| G: -5313.11806 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11578.53074 HOMO: -6.75931 LUMO: -1.49663 factor:1 | 1 (-1.04699) | -1 | -1 |
| G: -5313.11806 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11579.08836 HOMO: -6.84638 LUMO: -0.77552 factor:1 | 1 (-1.60460) | -1 | -1 |
| G: -5313.11806 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11578.82120 HOMO: -6.65863 LUMO: -1.34696 factor:1 | 1 (-1.33744) | -1 | -1 |
| G: -5313.11806 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11578.27542 HOMO: -6.25590 LUMO: -2.36467 factor:1 | 1 (-0.79166) | -1 | -1 |
| G: -5313.11806 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11578.38184 HOMO: -7.24911 LUMO: 0.33470 factor:1 | 1 (-0.89808) | 1 | 1 |
| G: -5313.11806 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11578.16682 HOMO: -6.65863 LUMO: -0.75648 factor:1 | 1 (-0.68306) | -1 | -1 |
| G: -5313.11806 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11579.02120 HOMO: -6.31576 LUMO: -0.83267 factor:1 | 1 (-1.53744) | -1 | -1 |
| G: -5313.11806 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11578.83913 HOMO: -6.64774 LUMO: -0.66124 factor:1 | 1 (-1.35537) | -1 | -1 |
| G: -5313.11806 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11578.03351 HOMO: -6.75387 LUMO: -1.00138 factor:1 | 1 (-0.54975) | -1 | -1 |
| G: -5313.11806 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11578.23299 HOMO: -6.52529 LUMO: -0.68301 factor:1 | 1 (-0.74924) | -1 | -1 |
| G: -5313.11806 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.84477 HOMO: -6.59332 LUMO: -0.68028 factor:1 | 1 (-0.36101) | -1 | -1 |
| G: -5313.11806 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.79947 HOMO: -5.98650 LUMO: 0.31565 factor:1 | -1 (0.68428) | -1 | -1 |
| G: -5313.11806 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.84769 HOMO: -6.59876 LUMO: 0.22585 factor:1 | -1 (0.63607) | -1 | -1 |
| G: -5313.11806 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.86249 HOMO: -6.72121 LUMO: 0.10340 factor:1 | -1 (0.62126) | -1 | -1 |
| G: -5313.11806 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.62652 HOMO: -6.09807 LUMO: 0.20136 factor:1 | -1 (0.85724) | -1 | -1 |
| G: -5313.11806 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.73604 HOMO: -6.31576 LUMO: 0.06259 factor:1 | -1 (0.74771) | -1 | -1 |
| G: -5313.11806 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.66398 HOMO: -6.35658 LUMO: -0.58232 factor:1 | 1 (-0.18022) | -1 | -1 |
| G: -5313.11806 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.89965 HOMO: -6.34842 LUMO: -0.55783 factor:1 | 1 (-0.41590) | -1 | -1 |
| G: -5313.11806 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.91835 HOMO: -6.47359 LUMO: -0.57144 factor:1 | 1 (-0.43459) | -1 | -1 |
| G: -5313.11806 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.59715 HOMO: -6.42189 LUMO: -0.09796 factor:1 | 1 (-0.11339) | -1 | -1 |
| G: -5313.11806 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.86385 HOMO: -6.35658 LUMO: -0.31293 factor:1 | -1 (0.61990) | -1 | -1 |
| G: -5313.11806 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.86021 HOMO: -7.35524 LUMO: 0.10340 factor:1 | -1 (0.62355) | 1 | 1 |
| G: -5313.11806 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.02035 HOMO: -7.10217 LUMO: 0.36463 factor:1 | -1 (0.46341) | 1 | 1 |
| G: -5313.11806 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.22378 HOMO: -6.43549 LUMO: -0.56872 factor:1 | -1 (0.25998) | -1 | -1 |
| G: -5313.11806 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.09305 HOMO: -6.50080 LUMO: -0.71294 factor:1 | -1 (0.39070) | -1 | -1 |
| G: -5313.11806 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.71770 HOMO: -6.59060 LUMO: -0.57960 factor:1 | -1 (0.76605) | -1 | -1 |
| G: -5313.11806 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.80674 HOMO: -6.78924 LUMO: -0.31565 factor:1 | -1 (0.67702) | -1 | -1 |
| G: -5313.11806 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.72845 HOMO: -6.35658 LUMO: 0.07891 factor:1 | -1 (0.75531) | -1 | -1 |
| G: -5313.11806 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.05586 HOMO: -6.74026 LUMO: -0.87621 factor:1 | -1 (0.42790) | -1 | -1 |
| G: -5313.11806 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.82402 HOMO: -6.54434 LUMO: 0.81906 factor:1 | -1 (0.65974) | -1 | -1 |
| G: -5313.11806 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.98347 HOMO: -6.66135 LUMO: 1.40955 factor:1 | -1 (0.50028) | -1 | -1 |
| G: -5313.11806 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.21616 HOMO: -6.73754 LUMO: -2.54971 factor:1 | -1 (0.26760) | -1 | -1 |
| G: -5313.11806 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.55585 HOMO: -6.65318 LUMO: 0.69389 factor:1 | -1 (0.92791) | -1 | -1 |
| G: -5313.11806 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.69454 HOMO: -6.73482 LUMO: 0.62858 factor:1 | -1 (0.78921) | -1 | -1 |
| G: -5313.11806 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.89047 HOMO: -6.83550 LUMO: 0.68573 factor:1 | -1 (0.59329) | -1 | -1 |
| G: -5313.11806 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.68799 HOMO: -6.83278 LUMO: 0.45987 factor:1 | -1 (0.79577) | -1 | -1 |
| G: -5313.11806 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.13257 HOMO: -6.78380 LUMO: 0.68301 factor:1 | -1 (0.35119) | -1 | -1 |
| G: -5313.11806 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.19061 HOMO: -6.90625 LUMO: 1.36601 factor:1 | -1 (0.29315) | -1 | -1 |
| G: -5313.11806 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.92418 HOMO: -6.82734 LUMO: 1.48302 factor:1 | -1 (0.55957) | -1 | -1 |
| G: -5313.11806 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.76323 HOMO: -6.44094 LUMO: -0.94424 factor:1 | -1 (0.72053) | -1 | -1 |
| G: -5313.11806 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.61057 HOMO: -6.91441 LUMO: 0.28844 factor:1 | -1 (0.87319) | -1 | -1 |
| G: -5313.11806 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11578.08398 HOMO: -6.49808 LUMO: -0.51157 factor:1 | 1 (-0.60023) | -1 | -1 |
| G: -5313.11806 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11579.01891 HOMO: -7.09673 LUMO: -0.06259 factor:1 | 1 (-1.53516) | 1 | 1 |
| G: -5313.11806 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11578.31131 HOMO: -6.77019 LUMO: 0.92247 factor:1 | 1 (-0.82755) | -1 | -1 |
| G: -5313.11806 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11578.02292 HOMO: -6.75931 LUMO: 1.13744 factor:1 | 1 (-0.53917) | -1 | -1 |
| G: -5313.11806 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.78320 HOMO: -6.15794 LUMO: 1.12383 factor:1 | -1 (0.70056) | -1 | -1 |
| G: -5313.11806 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.75087 HOMO: -6.59604 LUMO: 1.19458 factor:1 | -1 (0.73288) | -1 | -1 |
| G: -5313.11806 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.07145 HOMO: -7.09401 LUMO: 0.60137 factor:1 | -1 (0.41231) | 1 | 1 |
| G: -5313.11806 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.99123 HOMO: -6.34025 LUMO: 0.48164 factor:1 | -1 (0.49253) | -1 | -1 |
| G: -5313.11806 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.66284 HOMO: -6.72665 LUMO: -2.47624 factor:1 | -1 (0.82091) | -1 | -1 |
| G: -5313.11806 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.77301 HOMO: -6.48175 LUMO: 0.58232 factor:1 | 1 (-0.28926) | -1 | -1 |
| G: -5313.11806 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11578.40494 HOMO: -6.94162 LUMO: 0.28300 factor:1 | 1 (-0.92119) | -1 | -1 |
| G: -5313.11806 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.74382 HOMO: -6.65591 LUMO: 0.57144 factor:1 | 1 (-0.26006) | -1 | -1 |
| G: -5313.11806 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.99171 HOMO: -6.58788 LUMO: -1.03947 factor:1 | 1 (-0.50795) | -1 | -1 |
| G: -5313.11806 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.68654 HOMO: -7.18108 LUMO: 0.37824 factor:1 | 1 (-0.20278) | 1 | 1 |
| G: -5313.11806 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.69530 HOMO: -6.63958 LUMO: -1.52112 factor:1 | 1 (-0.21154) | -1 | -1 |
| G: -5313.11806 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.91348 HOMO: -6.12528 LUMO: -0.53606 factor:1 | 1 (-0.42972) | -1 | -1 |
| G: -5313.11806 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.92741 HOMO: -6.22324 LUMO: -0.87893 factor:1 | 1 (-0.44365) | -1 | -1 |
| G: -5313.11806 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.50670 HOMO: -6.62053 LUMO: -0.91974 factor:1 | 1 (-0.02294) | -1 | -1 |
| G: -5313.11806 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11578.06241 HOMO: -6.84366 LUMO: -0.83811 factor:1 | 1 (-0.57865) | -1 | -1 |
| G: -5313.11806 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.97402 HOMO: -7.26000 LUMO: 0.25851 factor:1 | 1 (-0.49027) | 1 | 1 |
| G: -5313.11806 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11578.26331 HOMO: -6.49536 LUMO: -0.63403 factor:1 | 1 (-0.77955) | -1 | -1 |
| G: -5313.11806 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.73931 HOMO: -6.45726 LUMO: -0.77825 factor:1 | -1 (0.74445) | -1 | -1 |
| G: -5313.11806 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.83144 HOMO: -6.74570 LUMO: -0.75103 factor:1 | -1 (0.65231) | -1 | -1 |
| G: -5313.11806 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.57781 HOMO: -7.20285 LUMO: 0.10612 factor:1 | -1 (0.90595) | 1 | 1 |
| G: -5313.11806 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.89564 HOMO: -6.45182 LUMO: -0.56600 factor:1 | -1 (0.58812) | -1 | -1 |
| G: -5313.11806 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.04369 HOMO: -6.83278 LUMO: -0.71838 factor:1 | -1 (0.44006) | -1 | -1 |
| G: -5313.11806 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.61098 HOMO: -7.01510 LUMO: -1.09662 factor:1 | -1 (0.87278) | -1 | -1 |
| G: -5313.11806 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11578.45460 HOMO: -6.48719 LUMO: 0.16871 factor:1 | 1 (-0.97085) | -1 | -1 |
| G: -5313.11806 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.63078 HOMO: -7.30898 LUMO: 0.26667 factor:1 | 1 (-0.14702) | 1 | 1 |
| G: -5313.11806 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.76730 HOMO: -6.68856 LUMO: -0.78641 factor:1 | 1 (-0.28354) | -1 | -1 |
| G: -5313.11806 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.91810 HOMO: -6.56883 LUMO: -1.00682 factor:1 | 1 (-0.43435) | -1 | -1 |
| G: -5313.11806 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11578.14880 HOMO: -6.41100 LUMO: -0.48980 factor:1 | 1 (-0.66505) | -1 | -1 |
| G: -5313.11806 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11578.33079 HOMO: -6.52257 LUMO: -0.59865 factor:1 | 1 (-0.84704) | -1 | -1 |
| G: -5313.11806 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11578.37721 HOMO: -6.63686 LUMO: -0.56055 factor:1 | 1 (-0.89346) | -1 | -1 |
| G: -5313.11806 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.91239 HOMO: -6.79740 LUMO: -0.75376 factor:1 | 1 (-0.42863) | -1 | -1 |
| G: -5313.11806 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.64634 HOMO: -5.89127 LUMO: 0.22313 factor:1 | 1 (-0.16259) | -1 | -1 |
| G: -5313.11806 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.88866 HOMO: -6.34842 LUMO: 0.11429 factor:1 | 1 (-0.40491) | -1 | -1 |
| G: -5313.11806 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.93949 HOMO: -6.13617 LUMO: 1.94834 factor:1 | 1 (-0.45574) | -1 | -1 |
| G: -5313.11806 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.66830 HOMO: -6.50080 LUMO: 1.74153 factor:1 | 1 (-0.18455) | -1 | -1 |
| G: -5313.11806 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11578.10924 HOMO: -6.33481 LUMO: 1.68438 factor:1 | 1 (-0.62548) | -1 | -1 |
| G: -5313.11806 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11578.33316 HOMO: -6.53073 LUMO: 1.95106 factor:1 | 1 (-0.84940) | -1 | -1 |
| G: -5313.11806 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11578.24845 HOMO: -6.46270 LUMO: 1.89935 factor:1 | 1 (-0.76469) | -1 | -1 |
| G: -5313.11806 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11578.01057 HOMO: -5.87222 LUMO: 1.91568 factor:1 | 1 (-0.52681) | -1 | -1 |
| G: -5313.11806 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.89724 HOMO: -6.07630 LUMO: 1.81500 factor:1 | -1 (0.58651) | -1 | -1 |
| G: -5313.11806 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.74214 HOMO: -6.20964 LUMO: 1.81500 factor:1 | -1 (0.74162) | -1 | -1 |
| G: -5313.11806 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.87251 HOMO: -6.15522 LUMO: 1.90752 factor:1 | -1 (0.61125) | -1 | -1 |
| G: -5313.11806 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.94647 HOMO: -6.11984 LUMO: 1.95378 factor:1 | -1 (0.53729) | -1 | -1 |
| G: -5313.11806 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.93477 HOMO: -6.58516 LUMO: 2.04358 factor:1 | -1 (0.54899) | -1 | -1 |
| G: -5313.11806 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.00935 HOMO: -7.37156 LUMO: 0.24490 factor:1 | -1 (0.47440) | 1 | 1 |
| G: -5313.11806 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.60404 HOMO: -6.36474 LUMO: -0.90070 factor:1 | -1 (0.87972) | -1 | -1 |
| G: -5313.11806 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.82151 HOMO: -6.43549 LUMO: -0.40817 factor:1 | -1 (0.66224) | -1 | -1 |
| G: -5313.11806 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.69709 HOMO: -7.32258 LUMO: 0.29388 factor:1 | 1 (-0.21334) | 1 | 1 |
| G: -5313.11806 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11578.51531 HOMO: -6.41372 LUMO: -0.20409 factor:1 | 1 (-1.03156) | -1 | -1 |
| G: -5313.11806 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.89508 HOMO: -7.18381 LUMO: 0.42722 factor:1 | 1 (-0.41133) | 1 | 1 |
| G: -5313.11806 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.93759 HOMO: -6.53890 LUMO: -0.54151 factor:1 | 1 (-0.45383) | -1 | -1 |
| G: -5313.11806 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.63894 HOMO: -6.61509 LUMO: 0.08708 factor:1 | 1 (-0.15519) | -1 | -1 |
| G: -5313.11806 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.71595 HOMO: -6.78108 LUMO: 2.03541 factor:1 | 1 (-0.23219) | -1 | -1 |
| G: -5313.11806 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.60123 HOMO: -6.50896 LUMO: 1.53472 factor:1 | 1 (-0.11747) | -1 | -1 |
| G: -5313.11806 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.75565 HOMO: -6.65591 LUMO: 1.80411 factor:1 | 1 (-0.27190) | -1 | -1 |
| G: -5313.11806 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.65124 HOMO: -6.64502 LUMO: 1.52112 factor:1 | 1 (-0.16749) | -1 | -1 |
| G: -5313.11806 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.98387 HOMO: -6.72938 LUMO: 1.48030 factor:1 | 1 (-0.50012) | -1 | -1 |
| G: -5313.11806 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.89887 HOMO: -6.16882 LUMO: 1.96466 factor:1 | -1 (0.58488) | -1 | -1 |
| G: -5313.11806 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.09417 HOMO: -6.22597 LUMO: 1.43132 factor:1 | -1 (0.38959) | -1 | -1 |
| G: -5313.11806 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.98334 HOMO: -6.57699 LUMO: 2.05718 factor:1 | -1 (0.50042) | -1 | -1 |
| G: -5313.11806 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.03205 HOMO: -6.52529 LUMO: 1.89663 factor:1 | -1 (0.45171) | -1 | -1 |
| G: -5313.11806 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.01289 HOMO: -6.30760 LUMO: 1.88031 factor:1 | -1 (0.47087) | -1 | -1 |
| G: -5313.11806 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.98630 HOMO: -6.14977 LUMO: 1.92657 factor:1 | -1 (0.49745) | -1 | -1 |
| G: -5313.11806 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.23306 HOMO: -6.20964 LUMO: 1.83949 factor:1 | -1 (0.25070) | -1 | -1 |
| G: -5313.11806 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.17899 HOMO: -6.31848 LUMO: 1.91296 factor:1 | -1 (0.30477) | -1 | -1 |
| G: -5313.11806 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.77172 HOMO: -5.80691 LUMO: 2.19868 factor:1 | -1 (0.71204) | -1 | -1 |
| G: -5313.11806 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.86576 HOMO: -6.00827 LUMO: 2.15514 factor:1 | -1 (0.61800) | -1 | -1 |
| G: -5313.11806 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.77947 HOMO: -6.51713 LUMO: 2.08711 factor:1 | -1 (0.70429) | -1 | -1 |
| G: -5313.11806 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.99703 HOMO: -6.32937 LUMO: 2.11705 factor:1 | -1 (0.48673) | -1 | -1 |
| G: -5313.11806 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.72744 HOMO: -6.26678 LUMO: 1.95922 factor:1 | -1 (0.75631) | -1 | -1 |
| G: -5313.11806 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.03088 HOMO: -6.43005 LUMO: 2.56603 factor:1 | -1 (0.45288) | -1 | -1 |
| G: -5313.11806 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.98870 HOMO: -6.41644 LUMO: 2.68304 factor:1 | -1 (0.49506) | -1 | -1 |
| G: -5313.11806 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.95659 HOMO: -5.97834 LUMO: 2.02997 factor:1 | -1 (0.52717) | -1 | -1 |
| G: -5313.11806 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.06827 HOMO: -6.14161 LUMO: 1.77690 factor:1 | -1 (0.41549) | -1 | -1 |
| G: -5313.11806 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.91120 HOMO: -6.21508 LUMO: 1.80411 factor:1 | -1 (0.57255) | -1 | -1 |
| G: -5313.11806 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.25461 HOMO: -6.46270 LUMO: 2.34562 factor:1 | -1 (0.22915) | -1 | -1 |
| G: -5313.11806 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.89262 HOMO: -6.39195 LUMO: -0.75920 factor:1 | -1 (0.59114) | -1 | -1 |
| G: -5313.11806 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.63503 HOMO: -7.08584 LUMO: -1.14016 factor:1 | -1 (0.84872) | -1 | -1 |
| G: -5313.11806 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.90687 HOMO: -6.70216 LUMO: -0.65035 factor:1 | -1 (0.57688) | -1 | -1 |
| G: -5313.11806 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.69424 HOMO: -6.79468 LUMO: -0.83811 factor:1 | -1 (0.78951) | -1 | -1 |
| G: -5313.11806 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.97615 HOMO: -6.99877 LUMO: -0.79729 factor:1 | -1 (0.50760) | -1 | -1 |
| G: -5313.11806 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.05997 HOMO: -7.08040 LUMO: -0.85444 factor:1 | -1 (0.42379) | -1 | -1 |
| G: -5313.11806 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.75988 HOMO: -7.39333 LUMO: 0.12789 factor:1 | -1 (0.72388) | 1 | 1 |
| G: -5313.11806 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.98138 HOMO: -7.05047 LUMO: 0.13878 factor:1 | -1 (0.50238) | -1 | -1 |
| G: -5313.11806 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.89180 HOMO: -6.90897 LUMO: -0.77552 factor:1 | -1 (0.59196) | -1 | -1 |
| G: -5313.11806 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.85800 HOMO: -7.25456 LUMO: 0.05170 factor:1 | -1 (0.62575) | 1 | 1 |
| G: -5313.11806 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.76976 HOMO: -6.84638 LUMO: -0.84355 factor:1 | -1 (0.71400) | -1 | -1 |
| G: -5313.11806 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.49481 HOMO: -6.78108 LUMO: -0.81634 factor:1 | -1 (0.98894) | -1 | -1 |
| G: -5313.11806 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.62687 HOMO: -6.74570 LUMO: -0.77280 factor:1 | -1 (0.85689) | -1 | -1 |
| G: -5313.11806 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.54031 HOMO: -7.28177 LUMO: -1.68438 factor:1 | -1 (0.94345) | -1 | -1 |
| G: -5313.11806 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.89172 HOMO: -7.22190 LUMO: -1.63540 factor:1 | -1 (0.59204) | -1 | -1 |
| G: -5313.11806 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.98587 HOMO: -7.15932 LUMO: -1.57554 factor:1 | -1 (0.49789) | -1 | -1 |
| G: -5313.11806 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.88747 HOMO: -6.57971 LUMO: -0.93063 factor:1 | -1 (0.59628) | -1 | -1 |
| G: -5313.11806 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.07205 HOMO: -6.88176 LUMO: 0.58232 factor:1 | -1 (0.41171) | -1 | -1 |
| G: -5313.11806 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.73454 HOMO: -6.85727 LUMO: 0.51430 factor:1 | -1 (0.74921) | -1 | -1 |
| G: -5313.11806 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.13338 HOMO: -6.83550 LUMO: 0.87893 factor:1 | -1 (0.35037) | -1 | -1 |
| G: -5313.11806 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.00307 HOMO: -7.06680 LUMO: 0.87621 factor:1 | -1 (0.48069) | 1 | 1 |
| G: -5313.11806 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.07828 HOMO: -6.52257 LUMO: 0.81362 factor:1 | -1 (0.40548) | -1 | -1 |
| G: -5313.11806 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.34928 HOMO: -6.95523 LUMO: 1.17009 factor:1 | -1 (0.13448) | -1 | -1 |
| G: -5313.11806 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.16389 HOMO: -7.21374 LUMO: 0.97145 factor:1 | -1 (0.31987) | 1 | 1 |
| G: -5313.11806 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.98269 HOMO: -6.81373 LUMO: -1.54561 factor:1 | -1 (0.50107) | -1 | -1 |
| G: -5313.11806 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.92598 HOMO: -6.86543 LUMO: -1.52656 factor:1 | -1 (0.55778) | -1 | -1 |
| G: -5313.11806 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.99847 HOMO: -6.90081 LUMO: -0.78097 factor:1 | -1 (0.48529) | -1 | -1 |
| G: -5313.11806 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.17564 HOMO: -6.64502 LUMO: -0.82723 factor:1 | -1 (0.30811) | -1 | -1 |
| G: -5313.11806 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.10756 HOMO: -6.65591 LUMO: -0.82178 factor:1 | -1 (0.37620) | -1 | -1 |
| G: -5313.11806 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.14965 HOMO: -6.79468 LUMO: -1.46397 factor:1 | -1 (0.33410) | -1 | -1 |
| G: -5313.11806 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.28718 HOMO: -7.25728 LUMO: 0.73743 factor:1 | -1 (0.19658) | 1 | -1 |
| G: -5313.11806 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.83634 HOMO: -7.00149 LUMO: 1.30070 factor:1 | -1 (0.64741) | -1 | -1 |
| G: -5313.11806 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.87689 HOMO: -7.07768 LUMO: 0.78097 factor:1 | -1 (0.60687) | 1 | -1 |
| G: -5313.11806 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.76159 HOMO: -6.86271 LUMO: 0.86260 factor:1 | -1 (0.72216) | -1 | -1 |
| G: -5313.11806 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.96622 HOMO: -6.94707 LUMO: 0.39729 factor:1 | -1 (0.51753) | -1 | -1 |
| G: -5313.11806 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.91131 HOMO: -6.79740 LUMO: 0.67484 factor:1 | -1 (0.57245) | -1 | -1 |
| G: -5313.11806 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.75297 HOMO: -6.91986 LUMO: -1.14288 factor:1 | -1 (0.73079) | -1 | -1 |
| G: -5313.11806 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.09314 HOMO: -6.31576 LUMO: 1.01771 factor:1 | -1 (0.39062) | -1 | -1 |
| G: -5313.11806 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.01210 HOMO: -6.81645 LUMO: 0.81362 factor:1 | -1 (0.47165) | -1 | -1 |
| G: -5313.11806 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.00995 HOMO: -6.92258 LUMO: -0.99594 factor:1 | -1 (0.47380) | -1 | -1 |
| G: -5313.11806 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.68614 HOMO: -6.81373 LUMO: 0.61770 factor:1 | -1 (0.79762) | -1 | -1 |
| G: -5313.11806 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.64532 HOMO: -7.18653 LUMO: 1.19186 factor:1 | -1 (0.83844) | 1 | 1 |
| G: -5313.11806 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.46450 HOMO: -7.00693 LUMO: 0.45715 factor:1 | -1 (1.01926) | -1 | -1 |
| G: -5313.11806 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.57027 HOMO: -7.11306 LUMO: 0.53334 factor:1 | -1 (0.91349) | 1 | 1 |
| G: -5313.11806 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.93199 HOMO: -6.63414 LUMO: -1.64357 factor:1 | -1 (0.55177) | -1 | -1 |
| G: -5313.11806 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.86516 HOMO: -6.22052 LUMO: -0.74015 factor:1 | -1 (0.61860) | -1 | -1 |
| G: -5313.11806 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.87806 HOMO: -6.81101 LUMO: -0.50069 factor:1 | -1 (0.60570) | -1 | -1 |
| G: -5313.11806 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.01920 HOMO: -6.71849 LUMO: -0.51974 factor:1 | -1 (0.46455) | -1 | -1 |
| G: -5313.11806 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.99382 HOMO: -6.72121 LUMO: -1.77690 factor:1 | -1 (0.48994) | -1 | -1 |
| G: -5313.11806 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.21148 HOMO: -6.94162 LUMO: -1.78779 factor:1 | -1 (0.27228) | -1 | -1 |
| G: -5313.11806 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.05012 HOMO: -6.91169 LUMO: 0.88981 factor:1 | -1 (0.43364) | -1 | -1 |
| G: -5313.11806 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.05969 HOMO: -6.97428 LUMO: 0.70750 factor:1 | -1 (0.42406) | -1 | -1 |
| G: -5313.11806 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.91713 HOMO: -6.74842 LUMO: 1.15921 factor:1 | -1 (0.56662) | -1 | -1 |
| G: -5313.11806 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.74649 HOMO: -7.25183 LUMO: -0.99594 factor:1 | -1 (0.73727) | -1 | -1 |
| G: -5313.11806 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.71291 HOMO: -6.43821 LUMO: -1.00410 factor:1 | -1 (0.77084) | -1 | -1 |
| G: -5313.11806 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.62253 HOMO: -6.52257 LUMO: -0.68573 factor:1 | 1 (-0.13878) | -1 | -1 |
| G: -5313.11806 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.46533 HOMO: -6.60148 LUMO: -0.52518 factor:1 | -1 (0.01842) | -1 | -1 |
| G: -5313.11806 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.58476 HOMO: -6.07086 LUMO: -1.39594 factor:1 | 1 (-0.10101) | -1 | -1 |
| G: -5313.11806 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.75299 HOMO: -6.78108 LUMO: -1.54833 factor:1 | 1 (-0.26923) | -1 | -1 |
| G: -5313.11806 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.85318 HOMO: -6.73482 LUMO: -1.01498 factor:1 | 1 (-0.36942) | -1 | -1 |
| G: -5313.11806 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.64346 HOMO: -6.85183 LUMO: 1.06669 factor:1 | 1 (-0.15970) | -1 | -1 |
| G: -5313.11806 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.48506 HOMO: -6.98516 LUMO: 1.43948 factor:1 | 1 (-0.00131) | -1 | -1 |
| G: -5313.11806 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.33309 HOMO: -6.94162 LUMO: 0.79185 factor:1 | -1 (0.15067) | -1 | -1 |
| G: -5313.11806 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.73184 HOMO: -6.67495 LUMO: -1.06669 factor:1 | 1 (-0.24809) | -1 | -1 |
| G: -5313.11806 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11578.19977 HOMO: -6.88720 LUMO: -1.00682 factor:1 | 1 (-0.71601) | -1 | -1 |
| G: -5313.11806 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11578.08622 HOMO: -6.85999 LUMO: -0.78097 factor:1 | 1 (-0.60246) | -1 | -1 |
| G: -5313.11806 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11578.23781 HOMO: -6.51713 LUMO: -0.89798 factor:1 | 1 (-0.75405) | -1 | -1 |
| G: -5313.11806 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11578.80296 HOMO: -6.63141 LUMO: -0.91430 factor:1 | 1 (-1.31921) | -1 | -1 |
| G: -5313.11806 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11579.10817 HOMO: -6.63414 LUMO: 0.04354 factor:1 | 1 (-1.62441) | -1 | -1 |
| G: -5313.11806 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11578.32276 HOMO: -6.65046 LUMO: -0.73743 factor:1 | 1 (-0.83901) | -1 | -1 |
| G: -5313.11806 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.77533 HOMO: -6.73754 LUMO: -0.71838 factor:1 | 1 (-0.29157) | -1 | -1 |
| G: -5313.11806 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.98591 HOMO: -6.65863 LUMO: -0.60137 factor:1 | 1 (-0.50216) | -1 | -1 |
| G: -5313.11806 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.87840 HOMO: -6.61509 LUMO: -0.47892 factor:1 | 1 (-0.39465) | -1 | -1 |
| G: -5313.11806 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.97277 HOMO: -6.82189 LUMO: -0.64763 factor:1 | 1 (-0.48902) | -1 | -1 |
| G: -5313.11806 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.69840 HOMO: -6.56883 LUMO: -0.51974 factor:1 | 1 (-0.21464) | -1 | -1 |
| G: -5313.11806 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.94856 HOMO: -6.97428 LUMO: -0.95512 factor:1 | -1 (0.53519) | -1 | -1 |
| G: -5313.11806 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.87166 HOMO: -6.70489 LUMO: -0.04082 factor:1 | -1 (0.61209) | -1 | -1 |
| G: -5313.11806 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.90965 HOMO: -6.74026 LUMO: 0.02177 factor:1 | -1 (0.57411) | -1 | -1 |
| G: -5313.11806 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.00655 HOMO: -6.50080 LUMO: -0.89525 factor:1 | -1 (0.47721) | -1 | -1 |
| G: -5313.11806 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.11714 HOMO: -6.46815 LUMO: -0.61226 factor:1 | -1 (0.36662) | -1 | -1 |
| G: -5313.11806 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.12220 HOMO: -6.57971 LUMO: -0.64219 factor:1 | -1 (0.36156) | -1 | -1 |
| G: -5313.11806 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.85648 HOMO: -7.17836 LUMO: 0.37280 factor:1 | -1 (0.62728) | 1 | 1 |
| G: -5313.11806 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.81740 HOMO: -6.67223 LUMO: 0.12245 factor:1 | -1 (0.66635) | -1 | -1 |
| G: -5313.11806 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.81618 HOMO: -6.55250 LUMO: 0.22858 factor:1 | -1 (0.66758) | -1 | -1 |
| G: -5313.11806 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.95885 HOMO: -6.97156 LUMO: -1.12927 factor:1 | -1 (0.52491) | -1 | -1 |
| G: -5313.11806 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.83052 HOMO: -6.78924 LUMO: -0.84900 factor:1 | -1 (0.65324) | -1 | -1 |
| G: -5313.11806 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.01050 HOMO: -6.65046 LUMO: -0.65307 factor:1 | -1 (0.47326) | -1 | -1 |
| G: -5313.11806 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.80295 HOMO: -7.41782 LUMO: 0.08980 factor:1 | -1 (0.68080) | 1 | 1 |
| G: -5313.11806 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.01471 HOMO: -6.56339 LUMO: -0.68573 factor:1 | -1 (0.46904) | -1 | -1 |
| G: -5313.11806 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.19855 HOMO: -6.31032 LUMO: -0.31837 factor:1 | -1 (0.28520) | -1 | -1 |
| G: -5313.11806 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.72736 HOMO: -6.72938 LUMO: -0.45987 factor:1 | -1 (0.75639) | -1 | -1 |
| G: -5313.11806 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.88973 HOMO: -6.59876 LUMO: -1.03131 factor:1 | -1 (0.59402) | -1 | -1 |
| G: -5313.11806 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.88704 HOMO: -7.29265 LUMO: 0.29660 factor:1 | -1 (0.59672) | 1 | 1 |
| G: -5313.11806 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.73245 HOMO: -6.42189 LUMO: -0.51157 factor:1 | -1 (0.75131) | -1 | -1 |
| G: -5313.11806 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.97768 HOMO: -6.27767 LUMO: -0.52790 factor:1 | -1 (0.50608) | -1 | -1 |
| G: -5313.11806 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.81076 HOMO: -6.41644 LUMO: -0.44627 factor:1 | -1 (0.67299) | -1 | -1 |
| G: -5313.11806 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.05297 HOMO: -6.23413 LUMO: -0.52790 factor:1 | -1 (0.43078) | -1 | -1 |
| G: -5313.11806 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.90119 HOMO: -6.63414 LUMO: -0.44082 factor:1 | -1 (0.58257) | -1 | -1 |
| G: -5313.11806 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.74421 HOMO: -7.03142 LUMO: 0.47076 factor:1 | -1 (0.73955) | -1 | -1 |
| G: -5313.11806 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.64317 HOMO: -6.62053 LUMO: -0.14422 factor:1 | -1 (0.84059) | -1 | -1 |
| G: -5313.11806 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.00709 HOMO: -6.22324 LUMO: 1.96194 factor:1 | -1 (0.47666) | -1 | -1 |
| G: -5313.11806 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11578.18804 HOMO: -6.17971 LUMO: 1.71704 factor:1 | 1 (-0.70429) | -1 | -1 |
| G: -5313.11806 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11578.94767 HOMO: -6.70761 LUMO: 1.68711 factor:1 | 1 (-1.46392) | -1 | -1 |
| G: -5313.11806 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11578.05460 HOMO: -6.52801 LUMO: 1.56193 factor:1 | 1 (-0.57084) | -1 | -1 |
| G: -5313.11806 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11578.37251 HOMO: -6.55794 LUMO: 1.52384 factor:1 | 1 (-0.88875) | -1 | -1 |
| G: -5313.11806 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11578.11675 HOMO: -6.47359 LUMO: 1.82316 factor:1 | 1 (-0.63299) | -1 | -1 |
| G: -5313.11806 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.80815 HOMO: -6.65863 LUMO: 1.83133 factor:1 | -1 (0.67560) | -1 | -1 |
| G: -5313.11806 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.66565 HOMO: -6.46270 LUMO: 1.90208 factor:1 | -1 (0.81811) | -1 | -1 |
| G: -5313.11806 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.82271 HOMO: -6.41917 LUMO: 2.03269 factor:1 | -1 (0.66105) | -1 | -1 |
| G: -5313.11806 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.76521 HOMO: -6.48992 LUMO: 1.87486 factor:1 | -1 (0.71854) | -1 | -1 |
| G: -5313.11806 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.98837 HOMO: -6.51985 LUMO: 1.69527 factor:1 | -1 (0.49538) | -1 | -1 |
| G: -5313.11806 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.71746 HOMO: -6.36202 LUMO: 2.05718 factor:1 | -1 (0.76630) | -1 | -1 |
| G: -5313.11806 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.72151 HOMO: -5.96474 LUMO: 1.88575 factor:1 | -1 (0.76225) | -1 | -1 |
| G: -5313.11806 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.47764 HOMO: -6.56339 LUMO: 2.04630 factor:1 | -1 (1.00611) | -1 | -1 |
| G: -5313.11806 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.97221 HOMO: -6.43277 LUMO: 1.98371 factor:1 | -1 (0.51155) | -1 | -1 |
| G: -5313.11806 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.79710 HOMO: -6.53345 LUMO: 2.06262 factor:1 | 1 (-0.31334) | -1 | -1 |
| G: -5313.11806 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11578.39194 HOMO: -5.81779 LUMO: 2.11432 factor:1 | 1 (-0.90818) | -1 | -1 |
| G: -5313.11806 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.66313 HOMO: -5.91848 LUMO: 1.86942 factor:1 | 1 (-0.17938) | -1 | -1 |
| G: -5313.11806 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.80635 HOMO: -6.48447 LUMO: 1.70343 factor:1 | 1 (-0.32259) | -1 | -1 |
| G: -5313.11806 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.96902 HOMO: -6.29671 LUMO: -0.89525 factor:1 | 1 (-0.48526) | -1 | -1 |
| G: -5313.11806 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.70898 HOMO: -6.63414 LUMO: -0.76192 factor:1 | 1 (-0.22523) | -1 | -1 |
| G: -5313.11806 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.65320 HOMO: -6.56883 LUMO: -0.86260 factor:1 | 1 (-0.16945) | -1 | -1 |
| G: -5313.11806 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.97879 HOMO: -6.93074 LUMO: -0.27483 factor:1 | 1 (-0.49503) | -1 | -1 |
| G: -5313.11806 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.60357 HOMO: -6.85999 LUMO: -0.01905 factor:1 | 1 (-0.11981) | -1 | -1 |
| G: -5313.11806 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.78003 HOMO: -6.26406 LUMO: 0.21769 factor:1 | 1 (-0.29628) | -1 | -1 |
| G: -5313.11806 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.99318 HOMO: -6.62325 LUMO: 0.31293 factor:1 | 1 (-0.50942) | -1 | -1 |
| G: -5313.11806 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.89133 HOMO: -6.59604 LUMO: 0.19592 factor:1 | 1 (-0.40757) | -1 | -1 |
| G: -5313.11806 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.64357 HOMO: -6.43277 LUMO: -0.27756 factor:1 | 1 (-0.15981) | -1 | -1 |
| G: -5313.11806 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.71337 HOMO: -6.54978 LUMO: -0.46531 factor:1 | 1 (-0.22961) | -1 | -1 |
| G: -5313.11806 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.56610 HOMO: -6.65046 LUMO: -0.15783 factor:1 | 1 (-0.08234) | -1 | -1 |
| G: -5313.11806 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11578.20581 HOMO: -7.28721 LUMO: 0.23946 factor:1 | 1 (-0.72205) | 1 | 1 |
| G: -5313.11806 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11578.78011 HOMO: -6.71849 LUMO: -0.56600 factor:1 | 1 (-1.29635) | -1 | -1 |
| G: -5313.11806 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11578.16317 HOMO: -6.85183 LUMO: -0.84355 factor:1 | 1 (-0.67941) | -1 | -1 |
| G: -5313.11806 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.93772 HOMO: -6.53345 LUMO: -0.84627 factor:1 | 1 (-0.45397) | -1 | -1 |
| G: -5313.11806 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.96855 HOMO: -6.60148 LUMO: -0.63130 factor:1 | 1 (-0.48480) | -1 | -1 |
| G: -5313.11806 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.74956 HOMO: -6.36202 LUMO: -0.60137 factor:1 | 1 (-0.26580) | -1 | -1 |
| G: -5313.11806 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.61415 HOMO: -6.28855 LUMO: -0.52790 factor:1 | 1 (-0.13040) | -1 | -1 |
| G: -5313.11806 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.65117 HOMO: -7.07224 LUMO: 0.41906 factor:1 | -1 (0.83259) | 1 | 1 |
| G: -5313.11806 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.87381 HOMO: -6.36202 LUMO: -0.24218 factor:1 | -1 (0.60994) | -1 | -1 |
| G: -5313.11806 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.86274 HOMO: -6.43549 LUMO: 0.14150 factor:1 | -1 (0.62102) | -1 | -1 |
| G: -5313.11806 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.77433 HOMO: -6.76747 LUMO: -0.40545 factor:1 | -1 (0.70943) | -1 | -1 |
| G: -5313.11806 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.75863 HOMO: -6.15249 LUMO: -0.51157 factor:1 | -1 (0.72513) | -1 | -1 |
| G: -5313.11806 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.69073 HOMO: -6.33753 LUMO: -0.02993 factor:1 | -1 (0.79302) | -1 | -1 |
| G: -5313.11806 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.88622 HOMO: -6.49808 LUMO: -0.83811 factor:1 | -1 (0.59753) | -1 | -1 |
| G: -5313.11806 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.68766 HOMO: -6.64502 LUMO: -0.46259 factor:1 | -1 (0.79610) | -1 | -1 |
| G: -5313.11806 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.96815 HOMO: -6.34570 LUMO: 0.22041 factor:1 | -1 (0.51560) | -1 | -1 |
| G: -5313.11806 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.72434 HOMO: -6.63414 LUMO: -0.13606 factor:1 | -1 (0.75942) | -1 | -1 |
| G: -5313.11806 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.81936 HOMO: -6.59604 LUMO: -0.79729 factor:1 | -1 (0.66439) | -1 | -1 |
| G: -5313.11806 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.56866 HOMO: -7.09401 LUMO: 0.31837 factor:1 | -1 (0.91509) | 1 | 1 |
| G: -5313.11806 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.96481 HOMO: -6.48719 LUMO: -0.31021 factor:1 | -1 (0.51895) | -1 | -1 |
| G: -5313.11806 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.69520 HOMO: -7.11306 LUMO: 0.39729 factor:1 | -1 (0.78856) | 1 | 1 |
| G: -5313.11806 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.60766 HOMO: -6.95251 LUMO: 0.41089 factor:1 | -1 (0.87610) | -1 | -1 |
| G: -5313.11806 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.55049 HOMO: -6.61509 LUMO: -0.41906 factor:1 | -1 (0.93327) | -1 | -1 |
| G: -5313.11806 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.70728 HOMO: -6.25318 LUMO: -0.47348 factor:1 | -1 (0.77648) | -1 | -1 |
| G: -5313.11806 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.79612 HOMO: -6.77019 LUMO: -0.10340 factor:1 | -1 (0.68763) | -1 | -1 |
| G: -5313.11806 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11578.01846 HOMO: -6.54706 LUMO: -0.46259 factor:1 | 1 (-0.53470) | -1 | -1 |
| G: -5313.11806 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11579.11029 HOMO: -6.34297 LUMO: -0.50341 factor:1 | 1 (-1.62653) | -1 | -1 |
| G: -5313.11806 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11578.18981 HOMO: -6.20692 LUMO: -0.51974 factor:1 | 1 (-0.70605) | -1 | -1 |
| G: -5313.11806 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.64992 HOMO: -7.03686 LUMO: 0.46804 factor:1 | -1 (0.83384) | -1 | -1 |
| G: -5313.11806 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.78140 HOMO: -6.47087 LUMO: 0.22585 factor:1 | -1 (0.70235) | -1 | -1 |
| G: -5313.11806 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.79923 HOMO: -6.41917 LUMO: 0.19320 factor:1 | -1 (0.68453) | -1 | -1 |
| G: -5313.11806 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.64826 HOMO: -6.61237 LUMO: -0.04354 factor:1 | -1 (0.83550) | -1 | -1 |
| G: -5313.11806 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.81841 HOMO: -6.56339 LUMO: 0.36735 factor:1 | -1 (0.66535) | -1 | -1 |
| G: -5313.11806 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11578.35662 HOMO: -6.54978 LUMO: 1.12655 factor:1 | 1 (-0.87286) | -1 | -1 |
| G: -5313.11806 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.73696 HOMO: -6.43277 LUMO: 1.17553 factor:1 | 1 (-0.25320) | -1 | -1 |
| G: -5313.11806 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.65111 HOMO: -6.29944 LUMO: 1.40955 factor:1 | 1 (-0.16735) | -1 | -1 |
| G: -5313.11806 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.76719 HOMO: -6.74842 LUMO: 0.74015 factor:1 | 1 (-0.28343) | -1 | -1 |
| G: -5313.11806 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.73451 HOMO: -6.15522 LUMO: 1.94289 factor:1 | 1 (-0.25075) | -1 | -1 |
| G: -5313.11806 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.85348 HOMO: -6.20147 LUMO: 1.40139 factor:1 | 1 (-0.36972) | -1 | -1 |
| G: -5313.11806 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11578.54348 HOMO: -6.41100 LUMO: 1.40139 factor:1 | 1 (-1.05972) | -1 | -1 |
| G: -5313.11806 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.61078 HOMO: -6.74570 LUMO: 1.80956 factor:1 | 1 (-0.12702) | -1 | -1 |
| G: -5313.11806 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.94834 HOMO: -6.60148 LUMO: -1.04764 factor:1 | -1 (0.53541) | -1 | -1 |
| G: -5313.11806 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.11657 HOMO: -6.82734 LUMO: -0.83267 factor:1 | -1 (0.36719) | -1 | -1 |
| G: -5313.11806 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.05782 HOMO: -7.01782 LUMO: -0.32382 factor:1 | -1 (0.42594) | -1 | -1 |
| G: -5313.11806 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.05474 HOMO: -6.54434 LUMO: 0.11157 factor:1 | -1 (0.42901) | -1 | -1 |
| G: -5313.11806 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.01033 HOMO: -6.53617 LUMO: 0.32926 factor:1 | -1 (0.47342) | -1 | -1 |
| G: -5313.11806 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.11205 HOMO: -6.62597 LUMO: -0.60137 factor:1 | -1 (0.37171) | -1 | -1 |
| G: -5313.11806 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.89569 HOMO: -6.60965 LUMO: -0.75376 factor:1 | -1 (0.58807) | -1 | -1 |
| G: -5313.11806 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.76061 HOMO: -6.29399 LUMO: 0.06803 factor:1 | -1 (0.72314) | -1 | -1 |
| G: -5313.11806 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.28996 HOMO: -6.60692 LUMO: -0.47076 factor:1 | -1 (0.19380) | -1 | -1 |
| G: -5313.11806 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.12642 HOMO: -7.33891 LUMO: 0.39184 factor:1 | -1 (0.35734) | 1 | 1 |
| G: -5313.11806 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.16683 HOMO: -6.60692 LUMO: 1.46125 factor:1 | -1 (0.31693) | -1 | -1 |
| G: -5313.11806 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.12282 HOMO: -6.21780 LUMO: 2.09256 factor:1 | -1 (0.36093) | -1 | -1 |
| G: -5313.11806 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.26968 HOMO: -6.28311 LUMO: 1.80411 factor:1 | -1 (0.21407) | -1 | -1 |
| G: -5313.11806 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.27975 HOMO: -6.51168 LUMO: 1.84765 factor:1 | -1 (0.20400) | -1 | -1 |
| G: -5313.11806 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.99694 HOMO: -6.66951 LUMO: 2.01636 factor:1 | -1 (0.48681) | -1 | -1 |
| G: -5313.11806 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.02563 HOMO: -6.75387 LUMO: 1.73881 factor:1 | -1 (0.45813) | -1 | -1 |
| G: -5313.11806 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.49426 HOMO: -6.77291 LUMO: 1.89935 factor:1 | 1 (-0.01050) | -1 | -1 |
| G: -5313.11806 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.27080 HOMO: -6.36474 LUMO: 1.61091 factor:1 | -1 (0.21296) | -1 | -1 |
| G: -5313.11806 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.21970 HOMO: -6.60420 LUMO: 1.40955 factor:1 | -1 (0.26406) | -1 | -1 |
| G: -5313.11806 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.41154 HOMO: -6.81645 LUMO: 1.59731 factor:1 | -1 (0.07222) | -1 | -1 |
| G: -5313.11806 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.12786 HOMO: -5.90215 LUMO: 2.12249 factor:1 | -1 (0.35590) | -1 | -1 |
| G: -5313.11806 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.03646 HOMO: -6.26950 LUMO: 1.62996 factor:1 | -1 (0.44730) | -1 | -1 |
| G: -5313.11806 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.04252 HOMO: -6.41100 LUMO: 1.80684 factor:1 | -1 (0.44123) | -1 | -1 |
| G: -5313.11806 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.17208 HOMO: -6.64230 LUMO: 2.23405 factor:1 | -1 (0.31168) | -1 | -1 |
| G: -5313.11806 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.27534 HOMO: -6.66951 LUMO: 2.21501 factor:1 | -1 (0.20841) | -1 | -1 |
| G: -5313.11806 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.19602 HOMO: -6.90897 LUMO: 2.00004 factor:1 | -1 (0.28773) | -1 | -1 |
| G: -5313.11806 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.34925 HOMO: -6.61781 LUMO: 1.42043 factor:1 | -1 (0.13451) | -1 | -1 |
| G: -5313.11806 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.23695 HOMO: -6.56611 LUMO: 1.60003 factor:1 | -1 (0.24681) | -1 | -1 |
| G: -5313.11806 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.24002 HOMO: -6.70489 LUMO: 1.78779 factor:1 | -1 (0.24373) | -1 | -1 |
| G: -5313.11806 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.05303 HOMO: -6.46815 LUMO: 1.59459 factor:1 | -1 (0.43073) | -1 | -1 |
| G: -5313.11806 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.00054 HOMO: -6.31304 LUMO: 1.36873 factor:1 | -1 (0.48322) | -1 | -1 |
| G: -5313.11806 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.78951 HOMO: -6.22597 LUMO: 1.54833 factor:1 | -1 (0.69424) | -1 | -1 |
| G: -5313.11806 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.03101 HOMO: -5.63004 LUMO: 1.96466 factor:1 | -1 (0.45274) | -1 | -1 |
| G: -5313.11806 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.20609 HOMO: -7.02598 LUMO: 1.79323 factor:1 | -1 (0.27766) | -1 | -1 |
| G: -5313.11806 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.03836 HOMO: -6.78924 LUMO: 2.10888 factor:1 | -1 (0.44540) | -1 | -1 |
| G: -5313.11806 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.91520 HOMO: -6.13345 LUMO: 2.07351 factor:1 | -1 (0.56855) | -1 | -1 |
| G: -5313.11806 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.18606 HOMO: -6.46270 LUMO: -0.37552 factor:1 | -1 (0.29769) | -1 | -1 |
| G: -5313.11806 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.73112 HOMO: -6.51985 LUMO: -0.49525 factor:1 | -1 (0.75264) | -1 | -1 |
| G: -5313.11806 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.61925 HOMO: -6.60965 LUMO: 1.90480 factor:1 | -1 (0.86451) | -1 | -1 |
| G: -5313.11806 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.08764 HOMO: -6.51168 LUMO: 1.92112 factor:1 | -1 (0.39612) | -1 | -1 |
| G: -5313.11806 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.22753 HOMO: -6.71305 LUMO: 1.91024 factor:1 | -1 (0.25622) | -1 | -1 |
| G: -5313.11806 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.01792 HOMO: -6.86815 LUMO: 2.02997 factor:1 | -1 (0.46583) | -1 | -1 |
| G: -5313.11806 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.30457 HOMO: -6.69944 LUMO: 1.95106 factor:1 | -1 (0.17919) | -1 | -1 |
| G: -5313.11806 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.11387 HOMO: -6.45182 LUMO: 1.66806 factor:1 | -1 (0.36988) | -1 | -1 |
| G: -5313.11806 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.87577 HOMO: -6.44638 LUMO: 2.16058 factor:1 | -1 (0.60798) | -1 | -1 |
| G: -5313.11806 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.67611 HOMO: -6.65591 LUMO: 1.95106 factor:1 | 1 (-0.19236) | -1 | -1 |
| G: -5313.11806 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.67802 HOMO: -6.35114 LUMO: 1.42316 factor:1 | 1 (-0.19426) | -1 | -1 |
| G: -5313.11806 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.99155 HOMO: -6.48719 LUMO: 1.59187 factor:1 | 1 (-0.50779) | -1 | -1 |
| G: -5313.11806 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.90575 HOMO: -7.05591 LUMO: 1.61908 factor:1 | 1 (-0.42199) | -1 | -1 |
| G: -5313.11806 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.85865 HOMO: -6.92258 LUMO: 1.87214 factor:1 | 1 (-0.37489) | -1 | -1 |
| G: -5313.11806 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.81416 HOMO: -5.85861 LUMO: 2.11705 factor:1 | 1 (-0.33040) | -1 | -1 |
| G: -5313.11806 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11578.01541 HOMO: -6.27767 LUMO: 1.75513 factor:1 | 1 (-0.53166) | -1 | -1 |
| G: -5313.11806 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11578.09452 HOMO: -6.16882 LUMO: 1.73881 factor:1 | 1 (-0.61076) | -1 | -1 |
| G: -5313.11806 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.90474 HOMO: -6.62053 LUMO: 1.39594 factor:1 | 1 (-0.42099) | -1 | -1 |
| G: -5313.11806 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.85944 HOMO: -5.46405 LUMO: 1.68166 factor:1 | 1 (-0.37568) | -1 | -1 |
| G: -5313.11806 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.87750 HOMO: -6.39740 LUMO: 1.68711 factor:1 | 1 (-0.39375) | -1 | -1 |
| G: -5313.11806 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.94532 HOMO: -6.99333 LUMO: 2.08439 factor:1 | 1 (-0.46156) | -1 | -1 |
| G: -5313.11806 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.53225 HOMO: -6.16882 LUMO: 1.71976 factor:1 | 1 (-0.04849) | -1 | -1 |
| G: -5313.11806 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.52909 HOMO: -7.19741 LUMO: 2.24766 factor:1 | 1 (-0.04533) | 1 | 1 |
| G: -5313.11806 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.18925 HOMO: -6.77291 LUMO: 2.17691 factor:1 | -1 (0.29451) | -1 | -1 |
| G: -5313.11806 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.09014 HOMO: -6.29944 LUMO: 2.16603 factor:1 | -1 (0.39361) | -1 | -1 |
| G: -5313.11806 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.02601 HOMO: -6.10079 LUMO: 1.83949 factor:1 | -1 (0.45775) | -1 | -1 |
| G: -5313.11806 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.12761 HOMO: -6.63686 LUMO: 2.05990 factor:1 | -1 (0.35614) | -1 | -1 |
| G: -5313.11806 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.23515 HOMO: -6.91713 LUMO: 1.87486 factor:1 | -1 (0.24860) | -1 | -1 |
| G: -5313.11806 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.42912 HOMO: -6.63958 LUMO: 1.79323 factor:1 | -1 (0.05464) | -1 | -1 |
| G: -5313.11806 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.25564 HOMO: -6.61781 LUMO: 1.70071 factor:1 | -1 (0.22811) | -1 | -1 |
| G: -5313.11806 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.07262 HOMO: -6.20420 LUMO: 1.82861 factor:1 | -1 (0.41114) | -1 | -1 |
| G: -5313.11806 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.96851 HOMO: -6.47903 LUMO: -2.16875 factor:1 | -1 (0.51525) | -1 | -1 |
| G: -5313.11806 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.64830 HOMO: -6.53073 LUMO: 2.18235 factor:1 | 1 (-0.16455) | -1 | -1 |
| G: -5313.11806 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.78792 HOMO: -7.01782 LUMO: 1.72520 factor:1 | 1 (-0.30417) | -1 | -1 |
| G: -5313.11806 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.77935 HOMO: -6.66135 LUMO: -0.75648 factor:1 | 1 (-0.29560) | -1 | -1 |
| G: -5313.11806 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.48000 HOMO: -7.56749 LUMO: 0.22585 factor:1 | -1 (0.00376) | 1 | 1 |
| G: -5313.11806 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.60520 HOMO: -6.45182 LUMO: -0.71294 factor:1 | 1 (-0.12144) | -1 | -1 |
| G: -5313.11806 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.52966 HOMO: -6.31032 LUMO: -0.34286 factor:1 | 1 (-0.04591) | -1 | -1 |
| G: -5313.11806 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.73465 HOMO: -6.41917 LUMO: 2.04085 factor:1 | 1 (-0.25089) | -1 | -1 |
| G: -5313.11806 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.79674 HOMO: -6.61781 LUMO: 1.98915 factor:1 | 1 (-0.31299) | -1 | -1 |
| G: -5313.11806 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.89661 HOMO: -5.86405 LUMO: 1.57282 factor:1 | 1 (-0.41285) | -1 | -1 |
| G: -5313.11806 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.76188 HOMO: -6.44094 LUMO: 1.80956 factor:1 | 1 (-0.27813) | -1 | -1 |
| G: -5313.11806 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.63121 HOMO: -6.59060 LUMO: 2.08167 factor:1 | 1 (-0.14746) | -1 | -1 |
| G: -5313.11806 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.66942 HOMO: -6.20147 LUMO: 1.69799 factor:1 | 1 (-0.18566) | -1 | -1 |
| G: -5313.11806 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.44680 HOMO: -6.50352 LUMO: -0.41361 factor:1 | -1 (0.03695) | -1 | -1 |
| G: -5313.11806 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.38041 HOMO: -6.10896 LUMO: -0.55783 factor:1 | -1 (0.10335) | -1 | -1 |
| G: -5313.11806 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.87582 HOMO: -6.74842 LUMO: -0.56872 factor:1 | 1 (-0.39206) | -1 | -1 |
| G: -5313.11806 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.78741 HOMO: -6.59060 LUMO: -0.22041 factor:1 | 1 (-0.30365) | -1 | -1 |
| G: -5313.11806 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.57883 HOMO: -6.22052 LUMO: -0.60137 factor:1 | 1 (-0.09508) | -1 | -1 |
| G: -5313.11806 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.53548 HOMO: -6.65863 LUMO: 0.07891 factor:1 | 1 (-0.05173) | -1 | -1 |
| G: -5313.11806 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.71884 HOMO: -6.57427 LUMO: 1.71160 factor:1 | 1 (-0.23508) | -1 | -1 |
| G: -5313.11806 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.56027 HOMO: -5.84773 LUMO: 1.99459 factor:1 | 1 (-0.07652) | -1 | -1 |
| G: -5313.11806 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.60539 HOMO: -6.02188 LUMO: 1.91296 factor:1 | 1 (-0.12163) | -1 | -1 |
| G: -5313.11806 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.86542 HOMO: -6.17698 LUMO: 2.00004 factor:1 | 1 (-0.38167) | -1 | -1 |
| G: -5313.11806 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.84153 HOMO: -6.02732 LUMO: 1.90752 factor:1 | 1 (-0.35778) | -1 | -1 |
| G: -5313.11806 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.79122 HOMO: -6.68584 LUMO: -0.50885 factor:1 | 1 (-0.30746) | -1 | -1 |
| G: -5313.11806 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.86757 HOMO: -6.61781 LUMO: -0.73471 factor:1 | 1 (-0.38382) | -1 | -1 |
| G: -5313.11806 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.44610 HOMO: -6.66407 LUMO: -0.79729 factor:1 | -1 (0.03766) | -1 | -1 |
| G: -5313.11806 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.48253 HOMO: -6.56339 LUMO: 0.23130 factor:1 | -1 (0.00122) | -1 | -1 |
| G: -5313.11806 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11578.00534 HOMO: -6.76747 LUMO: 0.08980 factor:1 | 1 (-0.52159) | -1 | -1 |
| G: -5313.11806 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.02437 HOMO: -6.70489 LUMO: -0.53334 factor:1 | -1 (0.45938) | -1 | -1 |
| G: -5313.11806 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.83112 HOMO: -7.28993 LUMO: 0.10885 factor:1 | -1 (0.65264) | 1 | 1 |
| G: -5313.11806 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.03741 HOMO: -6.22052 LUMO: 0.51974 factor:1 | -1 (0.44635) | -1 | -1 |
| G: -5313.11806 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.16111 HOMO: -6.81645 LUMO: 0.25307 factor:1 | -1 (0.32265) | -1 | -1 |
| G: -5313.11806 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.77963 HOMO: -6.80285 LUMO: 0.02721 factor:1 | -1 (0.70412) | -1 | -1 |
| G: -5313.11806 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.97368 HOMO: -6.51441 LUMO: 0.08163 factor:1 | -1 (0.51008) | -1 | -1 |
| G: -5313.11806 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.91398 HOMO: -6.73482 LUMO: -0.77008 factor:1 | -1 (0.56978) | -1 | -1 |
| G: -5313.11806 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.86132 HOMO: -6.29127 LUMO: -0.44355 factor:1 | -1 (0.62243) | -1 | -1 |
| G: -5313.11806 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.74589 HOMO: -6.72938 LUMO: -0.64763 factor:1 | -1 (0.73786) | -1 | -1 |
| G: -5313.11806 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.68246 HOMO: -6.49264 LUMO: -0.74559 factor:1 | -1 (0.80129) | -1 | -1 |
| G: -5313.11806 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.05036 HOMO: -6.67223 LUMO: -0.55239 factor:1 | -1 (0.43340) | -1 | -1 |
| G: -5313.11806 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.90026 HOMO: -6.33481 LUMO: 0.33198 factor:1 | -1 (0.58349) | -1 | -1 |
| G: -5313.11806 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.29856 HOMO: -6.76475 LUMO: -0.25307 factor:1 | -1 (0.18520) | -1 | -1 |
| G: -5313.11806 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.01833 HOMO: -6.65318 LUMO: 0.03810 factor:1 | -1 (0.46542) | -1 | -1 |
| G: -5313.11806 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.92728 HOMO: -6.09263 LUMO: 0.21497 factor:1 | -1 (0.55647) | -1 | -1 |
| G: -5313.11806 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.89828 HOMO: -6.32120 LUMO: -0.85444 factor:1 | -1 (0.58548) | -1 | -1 |
| G: -5313.11806 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.85180 HOMO: -6.57155 LUMO: -0.67484 factor:1 | -1 (0.63196) | -1 | -1 |
| G: -5313.11806 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.98070 HOMO: -6.53345 LUMO: -0.78913 factor:1 | -1 (0.50306) | -1 | -1 |
| G: -5313.11806 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.20810 HOMO: -7.07768 LUMO: 0.28844 factor:1 | -1 (0.27565) | 1 | 1 |
| G: -5313.11806 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.69237 HOMO: -6.75114 LUMO: 0.18776 factor:1 | -1 (0.79139) | -1 | -1 |
| G: -5313.11806 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.96824 HOMO: -6.77019 LUMO: -0.12245 factor:1 | -1 (0.51552) | -1 | -1 |
| G: -5313.11806 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.09997 HOMO: -6.43549 LUMO: 0.16327 factor:1 | -1 (0.38379) | -1 | -1 |
| G: -5313.11806 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.91844 HOMO: -6.69400 LUMO: -0.16327 factor:1 | -1 (0.56532) | -1 | -1 |
| G: -5313.11806 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.90443 HOMO: -6.38651 LUMO: -0.61770 factor:1 | -1 (0.57933) | -1 | -1 |
| G: -5313.11806 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.82214 HOMO: -6.34297 LUMO: -0.33198 factor:1 | -1 (0.66162) | -1 | -1 |
| G: -5313.11806 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.06573 HOMO: -7.51578 LUMO: 0.02177 factor:1 | -1 (0.41802) | 1 | 1 |
| G: -5313.11806 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.81558 HOMO: -6.47359 LUMO: -0.22585 factor:1 | -1 (0.66818) | -1 | -1 |
| G: -5313.11806 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.76570 HOMO: -6.68040 LUMO: -0.47076 factor:1 | -1 (0.71805) | -1 | -1 |
| G: -5313.11806 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.68400 HOMO: -6.75659 LUMO: -0.57688 factor:1 | 1 (-0.20025) | -1 | -1 |
| G: -5313.11806 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.88300 HOMO: -6.73754 LUMO: -0.61226 factor:1 | 1 (-0.39925) | -1 | -1 |
| G: -5313.11806 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.80422 HOMO: -7.37429 LUMO: 0.31293 factor:1 | 1 (-0.32047) | 1 | 1 |
| G: -5313.11806 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.33064 HOMO: -6.23413 LUMO: -0.90886 factor:1 | -1 (0.15312) | -1 | -1 |
| G: -5313.11806 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.75894 HOMO: -6.51985 LUMO: -0.68028 factor:1 | 1 (-0.27519) | -1 | -1 |
| G: -5313.11806 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.47532 HOMO: -6.52257 LUMO: -0.77280 factor:1 | -1 (0.00844) | -1 | -1 |
| G: -5313.11806 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.45513 HOMO: -7.29537 LUMO: 0.31837 factor:1 | -1 (0.02863) | 1 | 1 |
| G: -5313.11806 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.65290 HOMO: -6.08447 LUMO: 0.25851 factor:1 | 1 (-0.16915) | -1 | -1 |
| G: -5313.11806 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.93150 HOMO: -6.20964 LUMO: 0.13606 factor:1 | -1 (0.55226) | -1 | -1 |
| G: -5313.11806 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.92059 HOMO: -6.49808 LUMO: -0.14150 factor:1 | -1 (0.56317) | -1 | -1 |
| G: -5313.11806 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.20541 HOMO: -7.10761 LUMO: 0.28028 factor:1 | -1 (0.27835) | 1 | 1 |
| G: -5313.11806 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.73593 HOMO: -6.60965 LUMO: -0.62858 factor:1 | -1 (0.74782) | -1 | -1 |
| G: -5313.11806 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.74094 HOMO: -6.40012 LUMO: -0.26939 factor:1 | -1 (0.74282) | -1 | -1 |
| G: -5313.11806 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.04489 HOMO: -6.65318 LUMO: -0.73199 factor:1 | -1 (0.43887) | -1 | -1 |
| G: -5313.11806 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.92568 HOMO: -6.51441 LUMO: -0.44899 factor:1 | -1 (0.55808) | -1 | -1 |
| G: -5313.11806 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.98187 HOMO: -6.28583 LUMO: -0.48708 factor:1 | -1 (0.50189) | -1 | -1 |
| G: -5313.11806 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.27722 HOMO: -6.96884 LUMO: 0.19864 factor:1 | -1 (0.20653) | -1 | -1 |
| G: -5313.11806 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.82358 HOMO: -6.89809 LUMO: 0.34558 factor:1 | -1 (0.66018) | -1 | -1 |
| G: -5313.11806 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.57054 HOMO: -6.67495 LUMO: -0.15510 factor:1 | -1 (0.91321) | -1 | -1 |
| G: -5313.11806 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.08184 HOMO: -7.34980 LUMO: 0.19864 factor:1 | -1 (0.40191) | 1 | 1 |
| G: -5313.11806 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.70129 HOMO: -6.71305 LUMO: -0.81634 factor:1 | -1 (0.78246) | -1 | -1 |
| G: -5313.11806 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.94511 HOMO: -6.39468 LUMO: -0.47076 factor:1 | -1 (0.53865) | -1 | -1 |
| G: -5313.11806 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.06628 HOMO: -6.31304 LUMO: 1.39594 factor:1 | -1 (0.41748) | -1 | -1 |
| G: -5313.11806 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.78309 HOMO: -6.57155 LUMO: 1.55105 factor:1 | -1 (0.70067) | -1 | -1 |
| G: -5313.11806 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.83762 HOMO: -6.68312 LUMO: 1.69255 factor:1 | -1 (0.64613) | -1 | -1 |
| G: -5313.11806 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.66676 HOMO: -6.61509 LUMO: 1.73881 factor:1 | -1 (0.81699) | -1 | -1 |
| G: -5313.11806 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.03112 HOMO: -6.17971 LUMO: 1.90208 factor:1 | -1 (0.45263) | -1 | -1 |
| G: -5313.11806 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.22819 HOMO: -6.53073 LUMO: 1.73337 factor:1 | -1 (0.25557) | -1 | -1 |
| G: -5313.11806 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.85466 HOMO: -5.91303 LUMO: 1.90480 factor:1 | -1 (0.62910) | -1 | -1 |
| G: -5313.11806 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.01031 HOMO: -6.42733 LUMO: 1.80139 factor:1 | -1 (0.47345) | -1 | -1 |
| G: -5313.11806 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.97088 HOMO: -6.78924 LUMO: 2.31569 factor:1 | -1 (0.51288) | -1 | -1 |
| G: -5313.11806 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.19308 HOMO: -6.04093 LUMO: 1.91568 factor:1 | -1 (0.29067) | -1 | -1 |
| G: -5313.11806 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.08269 HOMO: -6.90081 LUMO: 2.36739 factor:1 | -1 (0.40107) | -1 | -1 |
| G: -5313.11806 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.92135 HOMO: -6.60965 LUMO: 2.18507 factor:1 | -1 (0.56240) | -1 | -1 |
| G: -5313.11806 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.92456 HOMO: -6.75387 LUMO: 2.48712 factor:1 | -1 (0.55919) | -1 | -1 |
| G: -5313.11806 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.84701 HOMO: -6.56883 LUMO: 1.71432 factor:1 | -1 (0.63675) | -1 | -1 |
| G: -5313.11806 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.89330 HOMO: -6.41644 LUMO: 1.72792 factor:1 | -1 (0.59046) | -1 | -1 |
| G: -5313.11806 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.72197 HOMO: -6.92530 LUMO: 2.54426 factor:1 | -1 (0.76178) | -1 | -1 |
| G: -5313.11806 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.94451 HOMO: -6.41644 LUMO: 2.70209 factor:1 | -1 (0.53925) | -1 | -1 |
| G: -5313.11806 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.79626 HOMO: -6.29671 LUMO: 2.14698 factor:1 | -1 (0.68750) | -1 | -1 |
| G: -5313.11806 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.07939 HOMO: -6.29127 LUMO: 1.87486 factor:1 | -1 (0.40436) | -1 | -1 |
| G: -5313.11806 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.96478 HOMO: -6.75931 LUMO: 2.78917 factor:1 | -1 (0.51898) | -1 | -1 |
| G: -5313.11806 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.76636 HOMO: -6.40828 LUMO: 1.86942 factor:1 | -1 (0.71740) | -1 | -1 |
| G: -5313.11806 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.13714 HOMO: -6.45726 LUMO: 1.97010 factor:1 | -1 (0.34662) | -1 | -1 |
| G: -5313.11806 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.75381 HOMO: -6.43277 LUMO: 1.22723 factor:1 | -1 (0.72995) | -1 | -1 |
| G: -5313.11806 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.68619 HOMO: -6.63414 LUMO: 1.62452 factor:1 | -1 (0.79757) | -1 | -1 |
| G: -5313.11806 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.49944 HOMO: -6.54162 LUMO: 2.16058 factor:1 | -1 (0.98432) | -1 | -1 |
| G: -5313.11806 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.92116 HOMO: -6.40284 LUMO: 1.88575 factor:1 | -1 (0.56260) | -1 | -1 |
| G: -5313.11806 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.03504 HOMO: -6.20964 LUMO: 1.84221 factor:1 | -1 (0.44872) | -1 | -1 |
| G: -5313.11806 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.07667 HOMO: -6.58516 LUMO: 1.69799 factor:1 | -1 (0.40708) | -1 | -1 |
| G: -5313.11806 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.74293 HOMO: -6.44094 LUMO: 2.05446 factor:1 | -1 (0.74083) | -1 | -1 |
| G: -5313.11806 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.64899 HOMO: -6.61509 LUMO: 2.16058 factor:1 | -1 (0.83476) | -1 | -1 |
| G: -5313.11806 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.11213 HOMO: -6.65591 LUMO: 1.69527 factor:1 | -1 (0.37163) | -1 | -1 |
| G: -5313.11806 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.13232 HOMO: -5.55112 LUMO: 1.80411 factor:1 | -1 (0.35144) | -1 | -1 |
| G: -5313.11806 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.21714 HOMO: -6.68312 LUMO: 2.38100 factor:1 | -1 (0.26662) | -1 | -1 |
| G: -5313.11806 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.27488 HOMO: -6.51168 LUMO: 2.14698 factor:1 | -1 (0.20887) | -1 | -1 |
| G: -5313.11806 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.01229 HOMO: -6.04637 LUMO: 1.48302 factor:1 | -1 (0.47146) | -1 | -1 |
| G: -5313.11806 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.12990 HOMO: -6.81645 LUMO: -0.74287 factor:1 | -1 (0.35386) | -1 | -1 |
| G: -5313.11806 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.98062 HOMO: -6.96884 LUMO: -0.97961 factor:1 | -1 (0.50314) | -1 | -1 |
| G: -5313.11806 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.63745 HOMO: -6.45998 LUMO: 0.09796 factor:1 | 1 (-0.15369) | -1 | -1 |
| G: -5313.11806 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.52874 HOMO: -6.44638 LUMO: 0.09524 factor:1 | 1 (-0.04498) | -1 | -1 |
| G: -5313.11806 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.70515 HOMO: -6.16338 LUMO: -0.54151 factor:1 | 1 (-0.22139) | -1 | -1 |
| G: -5313.11806 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.89748 HOMO: -6.35930 LUMO: -0.47892 factor:1 | 1 (-0.41372) | -1 | -1 |
| G: -5313.11806 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.57842 HOMO: -6.65318 LUMO: -0.00272 factor:1 | 1 (-0.09467) | -1 | -1 |
| G: -5313.11806 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.45472 HOMO: -6.50080 LUMO: 0.14694 factor:1 | -1 (0.02903) | -1 | -1 |
| G: -5313.11806 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.96644 HOMO: -6.60420 LUMO: 0.94968 factor:1 | -1 (0.51732) | -1 | -1 |
| G: -5313.11806 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.98712 HOMO: -6.60148 LUMO: -0.77552 factor:1 | -1 (0.49664) | -1 | -1 |
| G: -5313.11806 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.79120 HOMO: -6.81645 LUMO: -1.05580 factor:1 | -1 (0.69256) | -1 | -1 |
| G: -5313.11806 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.68412 HOMO: -6.57971 LUMO: -0.82178 factor:1 | -1 (0.79963) | -1 | -1 |
| G: -5313.11806 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.41359 HOMO: -6.09263 LUMO: -0.45171 factor:1 | -1 (1.07017) | -1 | -1 |
| G: -5313.11806 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.86970 HOMO: -6.74298 LUMO: -0.61770 factor:1 | -1 (0.61405) | -1 | -1 |
| G: -5313.11806 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.60431 HOMO: -6.72393 LUMO: 1.21091 factor:1 | -1 (0.87944) | -1 | -1 |
| G: -5313.11806 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.29957 HOMO: -6.30488 LUMO: 1.70071 factor:1 | -1 (1.18419) | -1 | -1 |
| G: -5313.11806 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.16326 HOMO: -6.38107 LUMO: 1.55649 factor:1 | -1 (0.32050) | -1 | -1 |
| G: -5313.11806 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.08745 HOMO: -6.17154 LUMO: 1.46669 factor:1 | -1 (0.39631) | -1 | -1 |
| G: -5313.11806 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.26451 HOMO: -6.86543 LUMO: 1.98643 factor:1 | -1 (0.21924) | -1 | -1 |
| G: -5313.11806 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.38332 HOMO: -6.69944 LUMO: 1.65173 factor:1 | -1 (0.10044) | -1 | -1 |
| G: -5313.11806 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.39948 HOMO: -6.77836 LUMO: 2.16331 factor:1 | -1 (0.08427) | -1 | -1 |
| G: -5313.11806 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.03632 HOMO: -6.42189 LUMO: 2.36467 factor:1 | -1 (0.44744) | -1 | -1 |
| G: -5313.11806 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.09812 HOMO: -7.00965 LUMO: 2.04358 factor:1 | -1 (0.38564) | -1 | -1 |
| G: -5313.11806 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.94685 HOMO: -6.36746 LUMO: 2.13881 factor:1 | -1 (0.53691) | -1 | -1 |
| G: -5313.11806 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.28601 HOMO: -6.37835 LUMO: 1.89935 factor:1 | -1 (0.19775) | -1 | -1 |
| G: -5313.11806 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.99713 HOMO: -7.03959 LUMO: 1.27349 factor:1 | -1 (0.48662) | -1 | -1 |
| G: -5313.11806 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.09074 HOMO: -6.67495 LUMO: -0.89253 factor:1 | -1 (0.39301) | -1 | -1 |
| G: -5313.11806 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.34656 HOMO: -6.71849 LUMO: -0.97961 factor:1 | -1 (0.13720) | -1 | -1 |
| G: -5313.11806 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.19115 HOMO: -6.47903 LUMO: 0.01633 factor:1 | -1 (0.29260) | -1 | -1 |
| G: -5313.11806 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.84086 HOMO: -6.38379 LUMO: 0.01088 factor:1 | -1 (0.64290) | -1 | -1 |
| G: -5313.11806 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.68709 HOMO: -6.49536 LUMO: -0.55239 factor:1 | -1 (0.79667) | -1 | -1 |
| G: -5313.11806 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.80132 HOMO: -6.53345 LUMO: -0.53879 factor:1 | -1 (0.68243) | -1 | -1 |
| G: -5313.11806 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.69625 HOMO: -6.16610 LUMO: 2.15514 factor:1 | 1 (-0.21249) | -1 | -1 |
| G: -5313.11806 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.81827 HOMO: -6.35114 LUMO: 1.98643 factor:1 | 1 (-0.33451) | -1 | -1 |
| G: -5313.11806 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.88526 HOMO: -6.43277 LUMO: 2.16058 factor:1 | 1 (-0.40150) | -1 | -1 |
| G: -5313.11806 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.88980 HOMO: -6.89809 LUMO: 2.20684 factor:1 | 1 (-0.40605) | -1 | -1 |
| G: -5313.11806 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11578.06652 HOMO: -6.54434 LUMO: 1.93473 factor:1 | 1 (-0.58276) | -1 | -1 |
| G: -5313.11806 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.83829 HOMO: -6.72938 LUMO: 2.03269 factor:1 | 1 (-0.35454) | -1 | -1 |
| G: -5313.11806 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.65535 HOMO: -6.90353 LUMO: 2.19868 factor:1 | 1 (-0.17160) | -1 | -1 |
| G: -5313.11806 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.04835 HOMO: -6.41372 LUMO: 2.02453 factor:1 | -1 (0.43541) | -1 | -1 |
| G: -5313.11806 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.15640 HOMO: -6.46543 LUMO: 1.90752 factor:1 | -1 (0.32735) | -1 | -1 |
| G: -5313.11806 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.17488 HOMO: -6.55522 LUMO: 2.11977 factor:1 | -1 (0.30888) | -1 | -1 |
| G: -5313.11806 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.31189 HOMO: -6.28855 LUMO: 2.02181 factor:1 | -1 (0.17187) | -1 | -1 |
| G: -5313.11806 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.35012 HOMO: -6.45726 LUMO: 1.52112 factor:1 | -1 (0.13364) | -1 | -1 |
| G: -5313.11806 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.09091 HOMO: -6.37291 LUMO: 2.11705 factor:1 | -1 (0.39285) | -1 | -1 |
| G: -5313.11806 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.99406 HOMO: -6.88448 LUMO: 2.24494 factor:1 | -1 (0.48970) | -1 | -1 |
| G: -5313.11806 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.75104 HOMO: -6.86271 LUMO: 2.41637 factor:1 | -1 (0.73272) | -1 | -1 |
| G: -5313.11806 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.06114 HOMO: -6.69400 LUMO: 2.34562 factor:1 | -1 (0.42262) | -1 | -1 |
| G: -5313.11806 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.94192 HOMO: -6.18243 LUMO: 2.53882 factor:1 | -1 (0.54183) | -1 | -1 |
| G: -5313.11806 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.88837 HOMO: -6.61237 LUMO: 2.54154 factor:1 | -1 (0.59539) | -1 | -1 |
| G: -5313.11806 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.07659 HOMO: -6.69672 LUMO: 2.16331 factor:1 | -1 (0.40716) | -1 | -1 |
| G: -5313.11806 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.91991 HOMO: -6.33481 LUMO: 2.34018 factor:1 | -1 (0.56385) | -1 | -1 |
| G: -5313.11806 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.06304 HOMO: -5.99739 LUMO: 2.37283 factor:1 | -1 (0.42072) | -1 | -1 |
| G: -5313.11806 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.96138 HOMO: -6.49808 LUMO: 2.47351 factor:1 | -1 (0.52238) | -1 | -1 |
| G: -5313.11806 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.70750 HOMO: -6.22052 LUMO: 1.86398 factor:1 | -1 (0.77626) | -1 | -1 |
| G: -5313.11806 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.84739 HOMO: -6.32665 LUMO: 2.28031 factor:1 | -1 (0.63637) | -1 | -1 |
| G: -5313.11806 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.58676 HOMO: -5.98378 LUMO: 2.16331 factor:1 | -1 (0.89700) | -1 | -1 |
| G: -5313.11806 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.81666 HOMO: -6.08991 LUMO: 2.30208 factor:1 | 1 (-0.33290) | -1 | -1 |
| G: -5313.11806 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.73437 HOMO: -7.07224 LUMO: 1.55105 factor:1 | 1 (-0.25062) | 1 | 1 |
| G: -5313.11806 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.79914 HOMO: -6.84638 LUMO: 1.76874 factor:1 | 1 (-0.31538) | -1 | -1 |
| G: -5313.11806 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.63399 HOMO: -6.68856 LUMO: 1.47758 factor:1 | 1 (-0.15023) | -1 | -1 |
| G: -5313.11806 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.89179 HOMO: -6.69672 LUMO: 1.71976 factor:1 | 1 (-0.40803) | -1 | -1 |
| G: -5313.11806 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.87125 HOMO: -6.86543 LUMO: 2.24766 factor:1 | 1 (-0.38749) | -1 | -1 |
| G: -5313.11806 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11578.06064 HOMO: -7.21646 LUMO: 1.71976 factor:1 | 1 (-0.57688) | 1 | 1 |
| G: -5313.11806 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.61208 HOMO: -6.94162 LUMO: 2.21773 factor:1 | 1 (-0.12833) | -1 | -1 |
| G: -5313.11806 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.62373 HOMO: -6.34842 LUMO: 2.04358 factor:1 | 1 (-0.13998) | -1 | -1 |
| G: -5313.11806 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.53227 HOMO: -6.53345 LUMO: 1.96738 factor:1 | 1 (-0.04852) | -1 | -1 |
| G: -5313.11806 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.94232 HOMO: -6.34842 LUMO: 1.88303 factor:1 | 1 (-0.45857) | -1 | -1 |
| G: -5313.11806 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.12125 HOMO: -6.38651 LUMO: 2.08983 factor:1 | -1 (0.36251) | -1 | -1 |
| G: -5313.11806 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.03354 HOMO: -6.01372 LUMO: 1.43676 factor:1 | -1 (0.45021) | -1 | -1 |
| G: -5313.11806 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.34838 HOMO: -6.30216 LUMO: 1.41771 factor:1 | -1 (0.13538) | -1 | -1 |
| G: -5313.11806 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.90081 HOMO: -6.52801 LUMO: 1.77146 factor:1 | -1 (0.58295) | -1 | -1 |
| G: -5313.11806 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.73860 HOMO: -6.53617 LUMO: 1.72792 factor:1 | -1 (0.74516) | -1 | -1 |
| G: -5313.11806 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.93972 HOMO: -6.56611 LUMO: 2.20412 factor:1 | -1 (0.54404) | -1 | -1 |
| G: -5313.11806 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.95477 HOMO: -6.66679 LUMO: -0.72927 factor:1 | -1 (0.52899) | -1 | -1 |
| G: -5313.11806 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.23238 HOMO: -6.85455 LUMO: -0.85444 factor:1 | -1 (0.25138) | -1 | -1 |
| G: -5313.11806 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.09940 HOMO: -7.21646 LUMO: 0.27211 factor:1 | -1 (0.38436) | 1 | 1 |
| G: -5313.11806 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.70935 HOMO: -6.57971 LUMO: -0.41361 factor:1 | -1 (0.77441) | -1 | -1 |
| G: -5313.11806 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.63765 HOMO: -7.03142 LUMO: -1.14288 factor:1 | -1 (0.84611) | -1 | -1 |
| G: -5313.11806 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.10530 HOMO: -6.29944 LUMO: 0.06803 factor:1 | -1 (0.37846) | -1 | -1 |
| G: -5313.11806 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.99441 HOMO: -6.47359 LUMO: 0.28028 factor:1 | -1 (0.48934) | -1 | -1 |
| G: -5313.11806 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.93267 HOMO: -6.42189 LUMO: 1.61364 factor:1 | -1 (0.55108) | -1 | -1 |
| G: -5313.11806 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.20152 HOMO: -6.41100 LUMO: 1.80956 factor:1 | -1 (0.28224) | -1 | -1 |
| G: -5313.11806 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.25621 HOMO: -6.83278 LUMO: 1.83949 factor:1 | -1 (0.22754) | -1 | -1 |
| G: -5313.11806 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.79329 HOMO: -6.78380 LUMO: -0.76192 factor:1 | -1 (0.69046) | -1 | -1 |
| G: -5313.11806 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.80742 HOMO: -6.95795 LUMO: 2.13609 factor:1 | -1 (0.67634) | -1 | -1 |
| G: -5313.11806 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.01920 HOMO: -6.57155 LUMO: 1.89119 factor:1 | -1 (0.46455) | -1 | -1 |
| G: -5313.11806 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.68891 HOMO: -6.65591 LUMO: 1.93745 factor:1 | -1 (0.79484) | -1 | -1 |
| G: -5313.11806 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.49084 HOMO: -6.44638 LUMO: 2.26943 factor:1 | -1 (0.99292) | -1 | -1 |
| G: -5313.11806 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.67669 HOMO: -5.88038 LUMO: 1.90480 factor:1 | -1 (0.80706) | -1 | -1 |
| G: -5313.11806 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.59922 HOMO: -6.22052 LUMO: 2.17691 factor:1 | -1 (0.88453) | -1 | -1 |
| G: -5313.11806 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.93433 HOMO: -6.04637 LUMO: 2.23950 factor:1 | -1 (0.54943) | -1 | -1 |
| G: -5313.11806 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.64290 HOMO: -6.44366 LUMO: 2.24766 factor:1 | -1 (0.84086) | -1 | -1 |
| G: -5313.11806 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.13787 HOMO: -6.81917 LUMO: 2.08439 factor:1 | -1 (0.34588) | -1 | -1 |
| G: -5313.11806 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.85610 HOMO: -6.48447 LUMO: 2.28576 factor:1 | -1 (0.62766) | -1 | -1 |
| G: -5313.11806 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.02211 HOMO: -6.54434 LUMO: 1.99187 factor:1 | -1 (0.46164) | -1 | -1 |
| G: -5313.11806 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.09765 HOMO: -6.17698 LUMO: -0.65852 factor:1 | -1 (0.38610) | -1 | -1 |
| G: -5313.11806 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.72420 HOMO: -6.08174 LUMO: -0.58504 factor:1 | -1 (0.75955) | -1 | -1 |
| G: -5313.11806 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.97920 HOMO: -6.55250 LUMO: -0.86804 factor:1 | -1 (0.50455) | -1 | -1 |
| G: -5313.11806 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.78480 HOMO: -6.57699 LUMO: -0.89525 factor:1 | -1 (0.69895) | -1 | -1 |
| G: -5313.11806 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.86992 HOMO: -6.63141 LUMO: -1.04220 factor:1 | -1 (0.61383) | -1 | -1 |
| G: -5313.11806 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.14786 HOMO: -6.69128 LUMO: -0.76736 factor:1 | -1 (0.33590) | -1 | -1 |
| G: -5313.11806 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.73572 HOMO: -6.25318 LUMO: -1.03131 factor:1 | -1 (0.74804) | -1 | -1 |
| G: -5313.11806 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.45800 HOMO: -6.69944 LUMO: 0.01905 factor:1 | -1 (1.02576) | -1 | -1 |
| G: -5313.11806 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.77854 HOMO: -6.28583 LUMO: 0.38368 factor:1 | 1 (-0.29478) | -1 | -1 |
| G: -5313.11806 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.95933 HOMO: -6.90081 LUMO: -0.83811 factor:1 | 1 (-0.47557) | -1 | -1 |
| G: -5313.11806 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.75620 HOMO: -6.78380 LUMO: -0.10068 factor:1 | 1 (-0.27244) | -1 | -1 |
| G: -5313.11806 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.81748 HOMO: -6.30488 LUMO: -0.98505 factor:1 | 1 (-0.33372) | -1 | -1 |
| G: -5313.11806 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.87786 HOMO: -6.29671 LUMO: -1.79051 factor:1 | 1 (-0.39410) | -1 | -1 |
| G: -5313.11806 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11578.09582 HOMO: -6.76747 LUMO: -0.22041 factor:1 | 1 (-0.61207) | -1 | -1 |
| G: -5313.11806 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11578.06219 HOMO: -6.22597 LUMO: -0.94968 factor:1 | 1 (-0.57843) | -1 | -1 |
| G: -5313.11806 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.79258 HOMO: -6.73482 LUMO: 0.05987 factor:1 | 1 (-0.30882) | -1 | -1 |
| G: -5313.11806 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.97930 HOMO: -6.28855 LUMO: 0.34831 factor:1 | 1 (-0.49555) | -1 | -1 |
| G: -5313.11806 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.65464 HOMO: -6.69400 LUMO: 0.25307 factor:1 | 1 (-0.17089) | -1 | -1 |
| G: -5313.11806 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.59236 HOMO: -6.70216 LUMO: 0.61226 factor:1 | 1 (-0.10860) | -1 | -1 |
| G: -5313.11806 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.58583 HOMO: -6.70216 LUMO: 0.17415 factor:1 | 1 (-0.10207) | -1 | -1 |
| G: -5313.11806 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.70866 HOMO: -6.70761 LUMO: 0.24762 factor:1 | 1 (-0.22490) | -1 | -1 |
| G: -5313.11806 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.61007 HOMO: -6.68856 LUMO: -0.84900 factor:1 | 1 (-0.12632) | -1 | -1 |
| G: -5313.11806 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.45736 HOMO: -6.71033 LUMO: -0.38640 factor:1 | -1 (0.02640) | -1 | -1 |
| G: -5313.11806 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.84159 HOMO: -6.24501 LUMO: -0.09252 factor:1 | 1 (-0.35783) | -1 | -1 |
| G: -5313.11806 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.73775 HOMO: -6.81645 LUMO: -0.07347 factor:1 | 1 (-0.25399) | -1 | -1 |
| G: -5313.11806 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.76866 HOMO: -6.49536 LUMO: 0.09796 factor:1 | 1 (-0.28490) | -1 | -1 |
| G: -5313.11806 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.69198 HOMO: -6.71033 LUMO: -0.26395 factor:1 | 1 (-0.20822) | -1 | -1 |
| G: -5313.11806 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.64398 HOMO: -6.70489 LUMO: -0.09252 factor:1 | 1 (-0.16022) | -1 | -1 |
| G: -5313.11806 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.45382 HOMO: -6.23685 LUMO: 0.39729 factor:1 | -1 (0.02993) | -1 | -1 |
| G: -5313.11806 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.45067 HOMO: -6.69400 LUMO: -0.05442 factor:1 | -1 (0.03309) | -1 | -1 |
| G: -5313.11806 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.73813 HOMO: -6.36202 LUMO: 0.09796 factor:1 | 1 (-0.25437) | -1 | -1 |
| G: -5313.11806 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.61706 HOMO: -6.54978 LUMO: 0.15510 factor:1 | 1 (-0.13331) | -1 | -1 |
| G: -5313.11806 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.77612 HOMO: -6.77836 LUMO: 0.25851 factor:1 | 1 (-0.29236) | -1 | -1 |
| G: -5313.11806 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.90036 HOMO: -5.70623 LUMO: 0.73471 factor:1 | 1 (-0.41661) | -1 | -1 |
| G: -5313.11806 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.63804 HOMO: -5.58378 LUMO: 0.89253 factor:1 | 1 (-0.15429) | -1 | -1 |
| G: -5313.11806 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.69415 HOMO: -5.68718 LUMO: 0.87893 factor:1 | 1 (-0.21040) | -1 | -1 |
| G: -5313.11806 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.90746 HOMO: -5.10486 LUMO: 1.11567 factor:1 | 1 (-0.42371) | -1 | -1 |
| G: -5313.11806 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.72390 HOMO: -4.59328 LUMO: 1.27621 factor:1 | 1 (-0.24014) | -1 | -1 |
| G: -5313.11806 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.56887 HOMO: -4.45450 LUMO: 1.82044 factor:1 | 1 (-0.08512) | -1 | -1 |
| G: -5313.11806 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.67791 HOMO: -4.64226 LUMO: 1.70615 factor:1 | 1 (-0.19415) | -1 | -1 |
| G: -5313.11806 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.82305 HOMO: -5.04227 LUMO: 1.04492 factor:1 | 1 (-0.33930) | -1 | -1 |
| G: -5313.11806 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.67788 HOMO: -4.85723 LUMO: 0.93607 factor:1 | 1 (-0.19413) | -1 | -1 |
| G: -5313.11806 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.51148 HOMO: -4.72934 LUMO: 1.00410 factor:1 | 1 (-0.02773) | -1 | -1 |
| G: -5313.11806 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.85220 HOMO: -4.56335 LUMO: 1.56738 factor:1 | 1 (-0.36844) | -1 | -1 |
| G: -5313.11806 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.90191 HOMO: -5.48854 LUMO: 0.33198 factor:1 | 1 (-0.41816) | -1 | -1 |
| G: -5313.11806 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.75690 HOMO: -4.97424 LUMO: 1.33608 factor:1 | 1 (-0.27315) | -1 | -1 |
| G: -5313.11806 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.96763 HOMO: -4.60145 LUMO: 1.74697 factor:1 | 1 (-0.48387) | -1 | -1 |
| G: -5313.11806 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.71554 HOMO: -5.60010 LUMO: 0.74831 factor:1 | 1 (-0.23179) | -1 | -1 |
| G: -5313.11806 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.29466 HOMO: -5.66541 LUMO: 0.66668 factor:1 | -1 (0.18909) | -1 | -1 |
| G: -5313.11806 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.44297 HOMO: -6.50080 LUMO: 0.07075 factor:1 | -1 (0.04079) | -1 | -1 |
| G: -5313.11806 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.58400 HOMO: -5.79603 LUMO: 0.22313 factor:1 | 1 (-0.10025) | -1 | -1 |
| G: -5313.11806 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.84418 HOMO: -4.68036 LUMO: 1.29798 factor:1 | -1 (0.63958) | -1 | -1 |
| G: -5313.11806 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.94143 HOMO: -4.84363 LUMO: 1.34424 factor:1 | -1 (0.54232) | -1 | -1 |
| G: -5313.11806 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.01006 HOMO: -4.62321 LUMO: 1.82861 factor:1 | -1 (0.47370) | -1 | -1 |
| G: -5313.11806 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.90769 HOMO: -5.83684 LUMO: 0.82178 factor:1 | -1 (0.57607) | -1 | -1 |
| G: -5313.11806 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.05496 HOMO: -5.27629 LUMO: 0.57960 factor:1 | -1 (0.42880) | -1 | -1 |
| G: -5313.11806 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.99221 HOMO: -5.15928 LUMO: -2.96876 factor:1 | -1 (0.49155) | -1 | -1 |
| G: -5313.11806 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.17472 HOMO: -5.08853 LUMO: 0.89253 factor:1 | -1 (0.30904) | -1 | -1 |
| G: -5313.11806 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.13744 HOMO: -6.42461 LUMO: 0.04354 factor:1 | -1 (0.34632) | -1 | -1 |
| G: -5313.11806 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.99251 HOMO: -6.42733 LUMO: -0.00544 factor:1 | -1 (0.49125) | -1 | -1 |
| G: -5313.11806 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.84116 HOMO: -5.87494 LUMO: 0.69933 factor:1 | -1 (0.64260) | -1 | -1 |
| G: -5313.11806 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.16936 HOMO: -5.07492 LUMO: 1.02587 factor:1 | -1 (0.31440) | -1 | -1 |
| G: -5313.11806 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.78358 HOMO: -4.44362 LUMO: 1.99187 factor:1 | -1 (0.70018) | -1 | -1 |
| G: -5313.11806 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.80780 HOMO: -5.82052 LUMO: 0.43810 factor:1 | -1 (0.67596) | -1 | -1 |
| G: -5313.11806 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.70978 HOMO: -5.75793 LUMO: 0.76464 factor:1 | -1 (0.77397) | -1 | -1 |
| G: -5313.11806 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.79713 HOMO: -5.09669 LUMO: 0.72382 factor:1 | -1 (0.68662) | -1 | -1 |
| G: -5313.11806 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.78929 HOMO: -6.75387 LUMO: -2.02453 factor:1 | -1 (0.69446) | -1 | -1 |
| G: -5313.11806 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.94217 HOMO: -5.02322 LUMO: 1.14832 factor:1 | -1 (0.54159) | -1 | -1 |
| G: -5313.11806 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.12008 HOMO: -5.75521 LUMO: 0.73471 factor:1 | -1 (0.36368) | -1 | -1 |
| G: -5313.11806 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.01882 HOMO: -5.89943 LUMO: 0.54967 factor:1 | -1 (0.46493) | -1 | -1 |
| G: -5313.11806 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.95409 HOMO: -5.80147 LUMO: 0.72382 factor:1 | -1 (0.52967) | -1 | -1 |
| G: -5313.11806 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.79112 HOMO: -6.16066 LUMO: 0.39457 factor:1 | -1 (0.69264) | -1 | -1 |
| G: -5313.11806 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.77260 HOMO: -5.98650 LUMO: 0.76736 factor:1 | 1 (-0.28885) | -1 | -1 |
| G: -5313.11806 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.95446 HOMO: -4.74839 LUMO: 1.88847 factor:1 | 1 (-0.47070) | -1 | -1 |
| G: -5313.11806 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.84308 HOMO: -5.62459 LUMO: 0.26939 factor:1 | 1 (-0.35933) | -1 | -1 |
| G: -5313.11806 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.64814 HOMO: -4.88172 LUMO: 1.30070 factor:1 | 1 (-0.16438) | -1 | -1 |
| G: -5313.11806 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.96434 HOMO: -5.09397 LUMO: 0.98505 factor:1 | 1 (-0.48058) | -1 | -1 |
| G: -5313.11806 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.87887 HOMO: -6.50080 LUMO: -0.28300 factor:1 | 1 (-0.39511) | -1 | -1 |
| G: -5313.11806 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11578.05479 HOMO: -5.04227 LUMO: 1.49935 factor:1 | 1 (-0.57103) | -1 | -1 |
| G: -5313.11806 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.74382 HOMO: -5.22731 LUMO: 0.88437 factor:1 | 1 (-0.26006) | -1 | -1 |
| G: -5313.11806 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.70240 HOMO: -4.95519 LUMO: 1.25717 factor:1 | 1 (-0.21864) | -1 | -1 |
| G: -5313.11806 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11578.05517 HOMO: -4.61233 LUMO: 1.27621 factor:1 | 1 (-0.57141) | -1 | -1 |
| G: -5313.11806 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.78167 HOMO: -4.70757 LUMO: 1.63813 factor:1 | 1 (-0.29791) | -1 | -1 |
| G: -5313.11806 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.89421 HOMO: -4.85179 LUMO: 1.11839 factor:1 | 1 (-0.41046) | -1 | -1 |
| G: -5313.11806 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.70341 HOMO: -4.97696 LUMO: 1.00138 factor:1 | 1 (-0.21965) | -1 | -1 |
| G: -5313.11806 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.61546 HOMO: -5.64636 LUMO: 0.81090 factor:1 | 1 (-0.13170) | -1 | -1 |
| G: -5313.11806 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.47061 HOMO: -4.37831 LUMO: 1.90208 factor:1 | -1 (0.01314) | -1 | -1 |
| G: -5313.11806 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.86670 HOMO: -4.67764 LUMO: 1.54561 factor:1 | 1 (-0.38295) | -1 | -1 |
| G: -5313.11806 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.66833 HOMO: -5.87766 LUMO: 0.42994 factor:1 | 1 (-0.18457) | -1 | -1 |
| G: -5313.11806 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.47921 HOMO: -6.03821 LUMO: 0.32382 factor:1 | -1 (0.00454) | -1 | -1 |
| G: -5313.11806 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.68082 HOMO: -5.99739 LUMO: 0.69389 factor:1 | 1 (-0.19706) | -1 | -1 |
| G: -5313.11806 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.72773 HOMO: -6.43821 LUMO: 0.15238 factor:1 | 1 (-0.24398) | -1 | -1 |
| G: -5313.11806 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.64346 HOMO: -6.63414 LUMO: -0.07347 factor:1 | 1 (-0.15970) | -1 | -1 |
| G: -5313.11806 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.81846 HOMO: -6.50080 LUMO: 0.10068 factor:1 | 1 (-0.33470) | -1 | -1 |
| G: -5313.11806 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.85870 HOMO: -6.49264 LUMO: 0.19592 factor:1 | 1 (-0.37495) | -1 | -1 |
| G: -5313.11806 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.66534 HOMO: -5.83956 LUMO: 0.12517 factor:1 | 1 (-0.18158) | -1 | -1 |
| G: -5313.11806 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.54071 HOMO: -6.50896 LUMO: 0.19048 factor:1 | 1 (-0.05695) | -1 | -1 |
| G: -5313.11806 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.36441 HOMO: -6.56611 LUMO: 0.04898 factor:1 | -1 (0.11935) | -1 | -1 |
| G: -5313.11806 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.77329 HOMO: -6.68040 LUMO: -0.08436 factor:1 | 1 (-0.28953) | -1 | -1 |
| G: -5313.11806 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.58389 HOMO: -6.73754 LUMO: -0.08708 factor:1 | 1 (-0.10014) | -1 | -1 |
| G: -5313.11806 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.74156 HOMO: -6.80285 LUMO: -0.10612 factor:1 | 1 (-0.25780) | -1 | -1 |
| G: -5313.11806 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.42620 HOMO: -6.35658 LUMO: 0.02177 factor:1 | -1 (0.05755) | -1 | -1 |
| G: -5313.11806 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.33679 HOMO: -5.74160 LUMO: 0.14694 factor:1 | -1 (0.14697) | -1 | -1 |
| G: -5313.11806 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.57853 HOMO: -4.78376 LUMO: 0.92791 factor:1 | 1 (-0.09478) | -1 | -1 |
| G: -5313.11806 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.45037 HOMO: -5.90215 LUMO: 0.36463 factor:1 | -1 (0.03339) | -1 | -1 |
| G: -5313.11806 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.77092 HOMO: -4.99329 LUMO: 0.85988 factor:1 | 1 (-0.28716) | -1 | -1 |
| G: -5313.11806 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.41891 HOMO: -4.93887 LUMO: 1.33608 factor:1 | -1 (0.06484) | -1 | -1 |
| G: -5313.11806 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.15923 HOMO: -5.19193 LUMO: 0.50341 factor:1 | -1 (0.32452) | -1 | -1 |
| G: -5313.11806 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.44599 HOMO: -6.64502 LUMO: -1.98643 factor:1 | -1 (0.03777) | -1 | -1 |
| G: -5313.11806 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.71337 HOMO: -5.15384 LUMO: 0.94968 factor:1 | 1 (-0.22961) | -1 | -1 |
| G: -5313.11806 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.48161 HOMO: -6.31032 LUMO: 0.08436 factor:1 | -1 (0.00215) | -1 | -1 |
| G: -5313.11806 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.53709 HOMO: -4.88716 LUMO: 0.82995 factor:1 | 1 (-0.05333) | -1 | -1 |
| G: -5313.11806 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.56223 HOMO: -5.57017 LUMO: 0.19320 factor:1 | 1 (-0.07848) | -1 | -1 |
| G: -5313.11806 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.74335 HOMO: -4.92254 LUMO: 0.93879 factor:1 | 1 (-0.25960) | -1 | -1 |
| G: -5313.11806 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.69473 HOMO: -4.77288 LUMO: 1.60003 factor:1 | 1 (-0.21097) | -1 | -1 |
| G: -5313.11806 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.60112 HOMO: -4.97696 LUMO: 0.89798 factor:1 | 1 (-0.11736) | -1 | -1 |
| G: -5313.11806 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.88172 HOMO: -5.00690 LUMO: 1.14288 factor:1 | 1 (-0.39797) | -1 | -1 |
| G: -5313.11806 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.58727 HOMO: -4.88444 LUMO: 1.48574 factor:1 | 1 (-0.10351) | -1 | -1 |
| G: -5313.11806 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.75617 HOMO: -5.03955 LUMO: 1.51023 factor:1 | 1 (-0.27241) | -1 | -1 |
| G: -5313.11806 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.61453 HOMO: -5.22459 LUMO: 0.99049 factor:1 | 1 (-0.13078) | -1 | -1 |
| G: -5313.11806 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.53644 HOMO: -5.29534 LUMO: 0.96056 factor:1 | 1 (-0.05268) | -1 | -1 |
| G: -5313.11806 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.42729 HOMO: -5.35520 LUMO: 0.68301 factor:1 | -1 (0.05646) | -1 | -1 |
| G: -5313.11806 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.44610 HOMO: -5.27357 LUMO: 1.18642 factor:1 | -1 (0.03766) | -1 | -1 |
| G: -5313.11806 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.71035 HOMO: -5.79875 LUMO: 0.61770 factor:1 | 1 (-0.22659) | -1 | -1 |
| G: -5313.11806 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.81843 HOMO: -7.64640 LUMO: -2.45175 factor:1 | 1 (-0.33467) | -1 | -1 |
| G: -5313.11806 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.60485 HOMO: -7.46953 LUMO: -1.29798 factor:1 | 1 (-0.12109) | 1 | 1 |
| G: -5313.11806 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.39369 HOMO: -7.95389 LUMO: -0.37280 factor:1 | -1 (0.09007) | 1 | 1 |
| G: -5313.11806 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.43410 HOMO: -7.23279 LUMO: -1.19186 factor:1 | -1 (0.04966) | 1 | 1 |
| G: -5313.11806 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.32702 HOMO: -7.14299 LUMO: -1.12927 factor:1 | -1 (0.15674) | 1 | 1 |
| G: -5313.11806 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.18974 HOMO: -6.93074 LUMO: 0.31565 factor:1 | -1 (0.29402) | -1 | -1 |
| G: -5313.11806 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.70643 HOMO: -6.63141 LUMO: 0.28028 factor:1 | 1 (-0.22267) | -1 | -1 |
| G: -5313.11806 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.48514 HOMO: -7.10489 LUMO: -1.07213 factor:1 | 1 (-0.00139) | 1 | 1 |
| G: -5313.11806 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.14612 HOMO: -7.00693 LUMO: -0.69389 factor:1 | -1 (0.33764) | -1 | -1 |
| G: -5313.11806 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.21548 HOMO: -8.50356 LUMO: -1.79595 factor:1 | -1 (0.26828) | -1 | -1 |
| G: -5313.11806 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.52841 HOMO: -7.79334 LUMO: -2.33746 factor:1 | 1 (-0.04465) | -1 | -1 |
| G: -5313.11806 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.30457 HOMO: -7.24367 LUMO: -0.85172 factor:1 | -1 (0.17919) | 1 | 1 |
| G: -5313.11806 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.37135 HOMO: -7.94028 LUMO: -0.20136 factor:1 | -1 (0.11241) | 1 | 1 |
| G: -5313.11806 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11578.10940 HOMO: -7.22462 LUMO: 0.84627 factor:1 | 1 (-0.62564) | 1 | 1 |
| G: -5313.11806 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11578.39055 HOMO: -6.54978 LUMO: 0.34831 factor:1 | 1 (-0.90679) | -1 | -1 |
| G: -5313.11806 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11578.98925 HOMO: -6.86815 LUMO: 0.32109 factor:1 | 1 (-1.50550) | -1 | -1 |
| G: -5313.11806 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.70591 HOMO: -7.17564 LUMO: -1.28438 factor:1 | 1 (-0.22215) | 1 | 1 |
| G: -5313.11806 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11578.13473 HOMO: -7.03142 LUMO: -1.12655 factor:1 | 1 (-0.65098) | -1 | -1 |
| G: -5313.11806 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.74743 HOMO: -7.39878 LUMO: 0.15783 factor:1 | 1 (-0.26368) | 1 | 1 |
| G: -5313.11806 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11578.17299 HOMO: -7.25728 LUMO: 0.42178 factor:1 | 1 (-0.68924) | 1 | 1 |
| G: -5313.11806 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.99476 HOMO: -6.86543 LUMO: 0.93879 factor:1 | 1 (-0.51100) | -1 | -1 |
| G: -5313.11806 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11578.38946 HOMO: -7.09673 LUMO: -0.69661 factor:1 | 1 (-0.90570) | 1 | 1 |
| G: -5313.11806 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11578.93761 HOMO: -7.74708 LUMO: 0.01088 factor:1 | 1 (-1.45385) | 1 | 1 |
| G: -5313.11806 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11578.19879 HOMO: -6.80557 LUMO: 0.46531 factor:1 | 1 (-0.71503) | -1 | -1 |
| G: -5313.11806 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11578.45123 HOMO: -7.29265 LUMO: 1.31975 factor:1 | 1 (-0.96747) | 1 | 1 |
| G: -5313.11806 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11579.10898 HOMO: -6.93618 LUMO: 0.29388 factor:1 | 1 (-1.62523) | -1 | -1 |
| G: -5313.11806 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11578.98863 HOMO: -6.53073 LUMO: 0.71022 factor:1 | 1 (-1.50487) | -1 | -1 |
| G: -5313.11806 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.81339 HOMO: -6.41917 LUMO: -1.24084 factor:1 | 1 (-0.32964) | -1 | -1 |
| G: -5313.11806 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.96306 HOMO: -6.67495 LUMO: -1.09118 factor:1 | 1 (-0.47930) | -1 | -1 |
| G: -5313.11806 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11578.29947 HOMO: -6.97156 LUMO: -0.53606 factor:1 | 1 (-0.81572) | -1 | -1 |
| G: -5313.11806 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11578.18761 HOMO: -6.85183 LUMO: -0.45715 factor:1 | 1 (-0.70385) | -1 | -1 |
| G: -5313.11806 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.91223 HOMO: -7.12666 LUMO: -0.67484 factor:1 | 1 (-0.42847) | 1 | 1 |
| G: -5313.11806 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.69005 HOMO: -7.49946 LUMO: -0.14694 factor:1 | -1 (0.79370) | 1 | 1 |
| G: -5313.11806 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.85564 HOMO: -7.44231 LUMO: 0.58232 factor:1 | -1 (0.62812) | 1 | 1 |
| G: -5313.11806 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.10307 HOMO: -7.36340 LUMO: -0.68301 factor:1 | -1 (0.38069) | 1 | 1 |
| G: -5313.11806 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.79169 HOMO: -6.13073 LUMO: -0.54967 factor:1 | -1 (0.69207) | -1 | -1 |
| G: -5313.11806 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.60589 HOMO: -7.81511 LUMO: -0.06531 factor:1 | -1 (0.87787) | 1 | 1 |
| G: -5313.11806 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.64028 HOMO: -7.26816 LUMO: -1.02587 factor:1 | -1 (0.84347) | 1 | 1 |
| G: -5313.11806 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.65004 HOMO: -7.98110 LUMO: -0.17960 factor:1 | 1 (-0.16629) | 1 | 1 |
| G: -5313.11806 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11578.51580 HOMO: -7.44776 LUMO: -1.00954 factor:1 | 1 (-1.03205) | 1 | 1 |
| G: -5313.11806 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.97723 HOMO: -7.47769 LUMO: -1.02859 factor:1 | 1 (-0.49348) | 1 | 1 |
| G: -5313.11806 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.83108 HOMO: -6.75659 LUMO: 0.39457 factor:1 | 1 (-0.34733) | -1 | -1 |
| G: -5313.11806 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.58085 HOMO: -6.71849 LUMO: 0.36735 factor:1 | 1 (-0.09709) | -1 | -1 |
| G: -5313.11806 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.70308 HOMO: -7.64096 LUMO: -1.43948 factor:1 | 1 (-0.21932) | 1 | 1 |
| G: -5313.11806 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.59279 HOMO: -7.83144 LUMO: -1.36601 factor:1 | 1 (-0.10904) | 1 | 1 |
| G: -5313.11806 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.80050 HOMO: -7.19469 LUMO: 0.35103 factor:1 | 1 (-0.31674) | 1 | 1 |
| G: -5313.11806 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.65772 HOMO: -7.03414 LUMO: 0.20409 factor:1 | 1 (-0.17396) | -1 | -1 |
| G: -5313.11806 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.96877 HOMO: -7.22734 LUMO: 0.31293 factor:1 | 1 (-0.48502) | 1 | 1 |
| G: -5313.11806 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.76395 HOMO: -6.93618 LUMO: 0.56055 factor:1 | 1 (-0.28020) | -1 | -1 |
| G: -5313.11806 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11578.12815 HOMO: -6.94707 LUMO: -0.88709 factor:1 | 1 (-0.64439) | -1 | -1 |
| G: -5313.11806 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.97669 HOMO: -6.86543 LUMO: -0.83267 factor:1 | 1 (-0.49293) | -1 | -1 |
| G: -5313.11806 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11578.22407 HOMO: -6.82189 LUMO: -1.15376 factor:1 | 1 (-0.74031) | -1 | -1 |
| G: -5313.11806 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11578.80087 HOMO: -6.65046 LUMO: -0.46531 factor:1 | 1 (-1.31711) | -1 | -1 |
| G: -5313.11806 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11578.38970 HOMO: -6.52529 LUMO: 0.20953 factor:1 | 1 (-0.90595) | -1 | -1 |
| G: -5313.11806 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11578.15218 HOMO: -6.80557 LUMO: 0.44355 factor:1 | 1 (-0.66842) | -1 | -1 |
| G: -5313.11806 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.71168 HOMO: -6.93074 LUMO: -0.81634 factor:1 | 1 (-0.22792) | -1 | -1 |
| G: -5313.11806 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.95879 HOMO: -7.43143 LUMO: -0.45987 factor:1 | 1 (-0.47503) | 1 | 1 |
| G: -5313.11806 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.95217 HOMO: -7.07224 LUMO: -0.68028 factor:1 | 1 (-0.46842) | 1 | 1 |
| G: -5313.11806 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.82006 HOMO: -6.68040 LUMO: -0.71566 factor:1 | 1 (-0.33631) | -1 | -1 |
| G: -5313.11806 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.56789 HOMO: -6.26406 LUMO: -1.09934 factor:1 | 1 (-0.08414) | -1 | -1 |
| G: -5313.11806 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.91496 HOMO: -5.94569 LUMO: -0.72110 factor:1 | -1 (0.56880) | -1 | -1 |
| G: -5313.11806 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.82407 HOMO: -6.12256 LUMO: -0.42178 factor:1 | -1 (0.65969) | -1 | -1 |
| G: -5313.11806 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.93324 HOMO: -6.09807 LUMO: 0.11429 factor:1 | -1 (0.55051) | -1 | -1 |
| G: -5313.11806 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.17480 HOMO: -7.35252 LUMO: -0.55783 factor:1 | -1 (0.30896) | 1 | 1 |
| G: -5313.11806 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.12565 HOMO: -7.57837 LUMO: -0.76736 factor:1 | -1 (0.35810) | 1 | 1 |
| G: -5313.11806 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.96225 HOMO: -6.16066 LUMO: 0.01905 factor:1 | -1 (0.52151) | -1 | -1 |
| G: -5313.11806 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.93771 HOMO: -6.13345 LUMO: -0.41906 factor:1 | -1 (0.54605) | -1 | -1 |
| G: -5313.11806 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.74475 HOMO: -6.10351 LUMO: -0.33742 factor:1 | -1 (0.73901) | -1 | -1 |
| G: -5313.11806 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.76276 HOMO: -7.24639 LUMO: -0.51702 factor:1 | -1 (0.72099) | 1 | 1 |
| G: -5313.11806 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.68878 HOMO: -6.98244 LUMO: -1.82044 factor:1 | -1 (0.79498) | -1 | -1 |
| G: -5313.11806 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.82366 HOMO: -6.37563 LUMO: -1.67622 factor:1 | -1 (0.66009) | -1 | -1 |
| G: -5313.11806 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.95049 HOMO: -5.79058 LUMO: -2.55243 factor:1 | -1 (0.53326) | -1 | -1 |
| G: -5313.11806 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.92440 HOMO: -6.34025 LUMO: -0.27483 factor:1 | -1 (0.55936) | -1 | -1 |
| G: -5313.11806 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.05412 HOMO: -6.05453 LUMO: -0.51157 factor:1 | -1 (0.42964) | -1 | -1 |
| G: -5313.11806 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.09031 HOMO: -7.53755 LUMO: -0.38912 factor:1 | -1 (0.39345) | 1 | 1 |
| G: -5313.11806 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.87694 HOMO: -7.00421 LUMO: -0.50885 factor:1 | -1 (0.60681) | -1 | -1 |
| G: -5313.11806 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.82834 HOMO: -7.52123 LUMO: -0.37552 factor:1 | -1 (0.65541) | 1 | 1 |
| G: -5313.11806 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.66026 HOMO: -6.70489 LUMO: -1.04764 factor:1 | -1 (0.82350) | -1 | -1 |
| G: -5313.11806 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.80815 HOMO: -7.06408 LUMO: -1.16737 factor:1 | -1 (0.67560) | 1 | 1 |
| G: -5313.11806 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.68761 HOMO: -6.71849 LUMO: -1.02315 factor:1 | -1 (0.79615) | -1 | -1 |
| G: -5313.11806 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.85621 HOMO: -6.16610 LUMO: -0.50885 factor:1 | -1 (0.62755) | -1 | -1 |
| G: -5313.11806 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.69539 HOMO: -6.48447 LUMO: 0.07619 factor:1 | -1 (0.78837) | -1 | -1 |
| G: -5313.11806 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.11999 HOMO: -7.06135 LUMO: 0.09796 factor:1 | -1 (0.36376) | 1 | 1 |
| G: -5313.11806 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.89506 HOMO: -6.47359 LUMO: 0.22585 factor:1 | -1 (0.58869) | -1 | -1 |
| G: -5313.11806 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.90440 HOMO: -6.10896 LUMO: -0.62314 factor:1 | -1 (0.57936) | -1 | -1 |
| G: -5313.11806 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.75476 HOMO: -6.88176 LUMO: -0.96600 factor:1 | -1 (0.72899) | -1 | -1 |
| G: -5313.11806 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.67280 HOMO: -6.67495 LUMO: 0.21769 factor:1 | -1 (0.81095) | -1 | -1 |
| G: -5313.11806 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.55190 HOMO: -6.84911 LUMO: 0.38368 factor:1 | -1 (0.93185) | -1 | -1 |
| G: -5313.11806 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.70110 HOMO: -6.83550 LUMO: 1.29798 factor:1 | -1 (0.78265) | -1 | -1 |
| G: -5313.11806 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.94277 HOMO: -6.67495 LUMO: 1.46941 factor:1 | -1 (0.54099) | -1 | -1 |
| G: -5313.11806 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11578.14483 HOMO: -6.81917 LUMO: 1.30887 factor:1 | 1 (-0.66107) | -1 | -1 |
| G: -5313.11806 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11579.07984 HOMO: -6.56611 LUMO: 0.66396 factor:1 | 1 (-1.59608) | -1 | -1 |
| G: -5313.11806 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11578.29335 HOMO: -6.76203 LUMO: 0.60137 factor:1 | 1 (-0.80959) | -1 | -1 |
| G: -5313.11806 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11578.20937 HOMO: -6.55794 LUMO: 0.34286 factor:1 | 1 (-0.72562) | -1 | -1 |
| G: -5313.11806 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.98635 HOMO: -6.83550 LUMO: 0.35919 factor:1 | 1 (-0.50259) | -1 | -1 |
| G: -5313.11806 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.75493 HOMO: -7.17836 LUMO: 0.63130 factor:1 | -1 (0.72883) | 1 | 1 |
| G: -5313.11806 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.73351 HOMO: -6.29944 LUMO: -0.69389 factor:1 | -1 (0.75025) | -1 | -1 |
| G: -5313.11806 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.96571 HOMO: -7.06680 LUMO: -0.95784 factor:1 | -1 (0.51805) | 1 | 1 |
| G: -5313.11806 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.84187 HOMO: -6.84638 LUMO: -0.87076 factor:1 | -1 (0.64189) | -1 | -1 |
| G: -5313.11806 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.59903 HOMO: -6.96339 LUMO: -1.05308 factor:1 | -1 (0.88472) | -1 | -1 |
| G: -5313.11806 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.50972 HOMO: -6.75387 LUMO: -1.04220 factor:1 | -1 (0.97403) | -1 | -1 |
| G: -5313.11806 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.69416 HOMO: -6.71849 LUMO: -0.84355 factor:1 | -1 (0.78959) | -1 | -1 |
| G: -5313.11806 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.87185 HOMO: -7.16748 LUMO: 0.51702 factor:1 | -1 (0.61190) | 1 | 1 |
| G: -5313.11806 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.73758 HOMO: -6.92530 LUMO: 0.71566 factor:1 | 1 (-0.25383) | -1 | -1 |
| G: -5313.11806 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11578.44568 HOMO: -7.11034 LUMO: 0.01905 factor:1 | 1 (-0.96192) | 1 | -1 |
| G: -5313.11806 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.76953 HOMO: -6.79468 LUMO: 0.77008 factor:1 | 1 (-0.28577) | -1 | -1 |
| G: -5313.11806 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.97966 HOMO: -6.52801 LUMO: 0.98233 factor:1 | 1 (-0.49590) | -1 | -1 |
| G: -5313.11806 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.87266 HOMO: -6.76475 LUMO: 0.53334 factor:1 | 1 (-0.38891) | -1 | -1 |
| G: -5313.11806 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.59456 HOMO: -5.29261 LUMO: 0.57416 factor:1 | 1 (-0.11080) | -1 | -1 |
| G: -5313.11806 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.75707 HOMO: -6.57971 LUMO: 0.12789 factor:1 | 1 (-0.27331) | -1 | -1 |
| G: -5313.11806 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.92602 HOMO: -6.99333 LUMO: 0.51430 factor:1 | 1 (-0.44227) | -1 | -1 |
| G: -5313.11806 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.78575 HOMO: -6.41917 LUMO: 0.19048 factor:1 | 1 (-0.30199) | -1 | -1 |
| G: -5313.11806 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.54844 HOMO: -6.16066 LUMO: 1.77146 factor:1 | 1 (-0.06468) | -1 | -1 |
| G: -5313.11806 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11578.10545 HOMO: -6.90353 LUMO: 1.65717 factor:1 | 1 (-0.62170) | -1 | -1 |
| G: -5313.11806 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.93704 HOMO: -5.94569 LUMO: 1.29526 factor:1 | 1 (-0.45329) | -1 | -1 |
| G: -5313.11806 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11578.16984 HOMO: -6.60420 LUMO: 1.33880 factor:1 | 1 (-0.68608) | -1 | -1 |
| G: -5313.11806 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.91927 HOMO: -6.23957 LUMO: 0.09524 factor:1 | 1 (-0.43552) | -1 | -1 |
| G: -5313.11806 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11578.07949 HOMO: -6.80013 LUMO: 1.34696 factor:1 | 1 (-0.59574) | -1 | -1 |
| G: -5313.11806 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.76567 HOMO: -7.53483 LUMO: -1.52384 factor:1 | -1 (0.71808) | -1 | -1 |
| G: -5313.11806 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.54853 HOMO: -7.62463 LUMO: -1.65717 factor:1 | -1 (0.93523) | -1 | -1 |
| G: -5313.11806 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.85596 HOMO: -7.62463 LUMO: -1.61364 factor:1 | -1 (0.62779) | -1 | -1 |
| G: -5313.11806 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.59808 HOMO: -8.04096 LUMO: -1.66806 factor:1 | -1 (0.88568) | -1 | -1 |
| G: -5313.11806 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.81115 HOMO: -7.18381 LUMO: -1.17553 factor:1 | -1 (0.67261) | 1 | 1 |
| G: -5313.11806 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.78461 HOMO: -7.69538 LUMO: -1.36601 factor:1 | -1 (0.69914) | 1 | 1 |
| G: -5313.11806 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.56692 HOMO: -7.95117 LUMO: -1.48302 factor:1 | -1 (0.91683) | -1 | -1 |
| G: -5313.11806 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.54436 HOMO: -6.98516 LUMO: 0.35919 factor:1 | -1 (0.93939) | -1 | -1 |
| G: -5313.11806 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.34899 HOMO: -7.91579 LUMO: -0.32109 factor:1 | -1 (1.13477) | 1 | 1 |
| G: -5313.11806 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.72344 HOMO: -6.75659 LUMO: -0.03537 factor:1 | -1 (0.76031) | -1 | -1 |
| G: -5313.11806 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.74235 HOMO: -7.78518 LUMO: -2.36467 factor:1 | 1 (-0.25859) | -1 | -1 |
| G: -5313.11806 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.55516 HOMO: -7.96477 LUMO: -2.75651 factor:1 | 1 (-0.07140) | -1 | -1 |
| G: -5313.11806 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11578.59292 HOMO: -7.60286 LUMO: -2.35106 factor:1 | 1 (-1.10916) | -1 | -1 |
| G: -5313.11806 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.58553 HOMO: -7.38245 LUMO: -1.21635 factor:1 | 1 (-0.10177) | 1 | 1 |
| G: -5313.11806 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.82621 HOMO: -7.91579 LUMO: -1.50479 factor:1 | 1 (-0.34246) | -1 | -1 |
| G: -5313.11806 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.78539 HOMO: -8.07362 LUMO: -0.28028 factor:1 | 1 (-0.30164) | 1 | 1 |
| G: -5313.11806 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.81100 HOMO: -7.38245 LUMO: -1.15921 factor:1 | 1 (-0.32724) | 1 | 1 |
| G: -5313.11806 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.61336 HOMO: -7.18653 LUMO: -0.94968 factor:1 | 1 (-0.12961) | 1 | 1 |
| G: -5313.11806 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.80537 HOMO: -6.88448 LUMO: 0.38096 factor:1 | 1 (-0.32161) | -1 | -1 |
| G: -5313.11806 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.02780 HOMO: -6.97972 LUMO: 0.43266 factor:1 | -1 (0.45595) | -1 | -1 |
| G: -5313.11806 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.89789 HOMO: -6.88992 LUMO: -0.43538 factor:1 | -1 (0.58586) | -1 | -1 |
| G: -5313.11806 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.94946 HOMO: -7.97021 LUMO: -0.17143 factor:1 | -1 (0.53430) | 1 | 1 |
| G: -5313.11806 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.06759 HOMO: -6.92530 LUMO: 0.77280 factor:1 | -1 (0.41617) | -1 | -1 |
| G: -5313.11806 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.90641 HOMO: -7.89674 LUMO: -0.09796 factor:1 | -1 (0.57734) | 1 | 1 |
| G: -5313.11806 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.71041 HOMO: -7.02870 LUMO: 0.88709 factor:1 | -1 (0.77335) | -1 | -1 |
| G: -5313.11806 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.81270 HOMO: -6.78380 LUMO: 0.22041 factor:1 | -1 (0.67106) | -1 | -1 |
| G: -5313.11806 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.96054 HOMO: -7.24911 LUMO: -0.82178 factor:1 | -1 (0.52322) | 1 | 1 |
| G: -5313.11806 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.21268 HOMO: -6.77019 LUMO: 0.52790 factor:1 | -1 (0.27108) | -1 | -1 |
| G: -5313.11806 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.08187 HOMO: -8.56070 LUMO: -1.83405 factor:1 | -1 (0.40188) | -1 | -1 |
| G: -5313.11806 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.20574 HOMO: -7.74164 LUMO: -2.36195 factor:1 | -1 (0.27802) | -1 | -1 |
| G: -5313.11806 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.07199 HOMO: -7.39878 LUMO: -2.41637 factor:1 | -1 (0.41176) | -1 | -1 |
| G: -5313.11806 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.04816 HOMO: -7.61647 LUMO: -2.34018 factor:1 | -1 (0.43560) | -1 | -1 |
| G: -5313.11806 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.85226 HOMO: -6.93346 LUMO: -0.57688 factor:1 | -1 (0.63149) | -1 | -1 |
| G: -5313.11806 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.98435 HOMO: -6.85183 LUMO: -1.00410 factor:1 | -1 (0.49941) | -1 | -1 |
| G: -5313.11806 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.01730 HOMO: -7.18925 LUMO: -1.12655 factor:1 | -1 (0.46646) | 1 | 1 |
| G: -5313.11806 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.18955 HOMO: -6.85183 LUMO: -1.60275 factor:1 | -1 (0.29421) | -1 | -1 |
| G: -5313.11806 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.97814 HOMO: -7.51578 LUMO: 0.12517 factor:1 | -1 (0.50561) | 1 | 1 |
| G: -5313.11806 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.21940 HOMO: -7.36068 LUMO: 0.05714 factor:1 | -1 (0.26436) | 1 | 1 |
| G: -5313.11806 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.05120 HOMO: -7.49674 LUMO: 0.18776 factor:1 | -1 (0.43255) | 1 | 1 |
| G: -5313.11806 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.80480 HOMO: -7.09401 LUMO: -1.24900 factor:1 | -1 (0.67895) | 1 | 1 |
| G: -5313.11806 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.98315 HOMO: -7.22462 LUMO: -1.61364 factor:1 | -1 (0.50061) | -1 | -1 |
| G: -5313.11806 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.86979 HOMO: -7.74436 LUMO: -0.18776 factor:1 | -1 (0.61397) | 1 | 1 |
| G: -5313.11806 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.76970 HOMO: -7.35252 LUMO: 0.75376 factor:1 | -1 (0.71405) | 1 | 1 |
| G: -5313.11806 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.98927 HOMO: -7.75252 LUMO: 0.00816 factor:1 | -1 (0.49449) | 1 | 1 |
| G: -5313.11806 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.84516 HOMO: -7.06680 LUMO: 0.24490 factor:1 | -1 (0.63860) | 1 | 1 |
| G: -5313.11806 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.12816 HOMO: -7.49129 LUMO: 0.14150 factor:1 | -1 (0.35560) | 1 | 1 |
| G: -5313.11806 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.92805 HOMO: -6.90625 LUMO: -1.11295 factor:1 | -1 (0.55571) | -1 | -1 |
| G: -5313.11806 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.12729 HOMO: -6.78380 LUMO: -0.93063 factor:1 | -1 (0.35647) | -1 | -1 |
| G: -5313.11806 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.93028 HOMO: -7.79878 LUMO: 0.30477 factor:1 | -1 (0.55348) | 1 | 1 |
| G: -5313.11806 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.77710 HOMO: -7.87498 LUMO: 0.61770 factor:1 | -1 (0.70665) | 1 | 1 |
| G: -5313.11806 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.84151 HOMO: -7.23823 LUMO: 0.30205 factor:1 | -1 (0.64224) | 1 | 1 |
| G: -5313.11806 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.59060 HOMO: -7.67633 LUMO: 0.13061 factor:1 | -1 (0.89316) | 1 | 1 |
| G: -5313.11806 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.63027 HOMO: -7.79606 LUMO: 0.34558 factor:1 | -1 (0.85349) | 1 | 1 |
| G: -5313.11806 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.60276 HOMO: -6.66135 LUMO: -2.60141 factor:1 | -1 (0.88100) | -1 | -1 |
| G: -5313.11806 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.47770 HOMO: -7.03142 LUMO: 0.50885 factor:1 | -1 (1.00606) | -1 | -1 |
| G: -5313.11806 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.97346 HOMO: -7.05591 LUMO: -0.06531 factor:1 | -1 (0.51030) | -1 | -1 |
| G: -5313.11806 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.07588 HOMO: -7.45592 LUMO: -1.39594 factor:1 | -1 (0.40787) | 1 | 1 |
| G: -5313.11806 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.02892 HOMO: -7.22462 LUMO: -1.10478 factor:1 | -1 (0.45484) | 1 | 1 |
| G: -5313.11806 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.90965 HOMO: -8.14709 LUMO: -0.55783 factor:1 | -1 (0.57411) | 1 | 1 |
| G: -5313.11806 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.13540 HOMO: -7.22190 LUMO: -1.14560 factor:1 | -1 (0.34836) | 1 | 1 |
| G: -5313.11806 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.24680 HOMO: -7.28721 LUMO: -1.14016 factor:1 | -1 (0.23696) | 1 | 1 |
| G: -5313.11806 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.13428 HOMO: -6.97156 LUMO: 0.51702 factor:1 | -1 (0.34948) | -1 | -1 |
| G: -5313.11806 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.15844 HOMO: -7.37156 LUMO: 0.29388 factor:1 | -1 (0.32531) | 1 | -1 |
| G: -5313.11806 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.02046 HOMO: -7.66273 LUMO: -1.59731 factor:1 | -1 (0.46330) | -1 | -1 |
| G: -5313.11806 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.83944 HOMO: -7.50490 LUMO: -1.49935 factor:1 | -1 (0.64431) | -1 | -1 |
| G: -5313.11806 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.77604 HOMO: -7.61102 LUMO: -1.45581 factor:1 | -1 (0.70771) | 1 | 1 |
| G: -5313.11806 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.79210 HOMO: -7.58653 LUMO: -1.61091 factor:1 | -1 (0.69166) | -1 | -1 |
| G: -5313.11806 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.98617 HOMO: -7.36068 LUMO: -1.14560 factor:1 | -1 (0.49759) | 1 | 1 |
| G: -5313.11806 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.66085 HOMO: -6.96339 LUMO: 0.26939 factor:1 | 1 (-0.17709) | -1 | -1 |
| G: -5313.11806 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.42819 HOMO: -6.53617 LUMO: 0.22313 factor:1 | -1 (0.05557) | -1 | -1 |
| G: -5313.11806 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.75987 HOMO: -7.33619 LUMO: -1.02587 factor:1 | 1 (-0.27611) | 1 | 1 |
| G: -5313.11806 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.91451 HOMO: -6.87904 LUMO: 0.33742 factor:1 | 1 (-0.43076) | -1 | -1 |
| G: -5313.11806 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.72196 HOMO: -6.88448 LUMO: 0.58777 factor:1 | 1 (-0.23821) | -1 | -1 |
| G: -5313.11806 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.96485 HOMO: -6.55522 LUMO: -1.51295 factor:1 | 1 (-0.48110) | -1 | -1 |
| G: -5313.11806 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.49037 HOMO: -7.43415 LUMO: 0.10612 factor:1 | 1 (-0.00661) | 1 | 1 |
| G: -5313.11806 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.46819 HOMO: -7.54300 LUMO: -0.02449 factor:1 | -1 (0.01556) | 1 | 1 |
| G: -5313.11806 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.34155 HOMO: -7.42054 LUMO: 0.28028 factor:1 | -1 (0.14221) | 1 | 1 |
| G: -5313.11806 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.64501 HOMO: -6.98244 LUMO: -0.95784 factor:1 | 1 (-0.16125) | -1 | -1 |
| G: -5313.11806 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.70632 HOMO: -6.96884 LUMO: -1.12383 factor:1 | 1 (-0.22256) | -1 | -1 |
| G: -5313.11806 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.79822 HOMO: -6.80829 LUMO: -0.98233 factor:1 | -1 (0.68554) | -1 | -1 |
| G: -5313.11806 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.84396 HOMO: -7.60830 LUMO: 0.58504 factor:1 | -1 (0.63979) | 1 | 1 |
| G: -5313.11806 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.08105 HOMO: -7.52123 LUMO: 0.08163 factor:1 | -1 (0.40270) | 1 | 1 |
| G: -5313.11806 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.68439 HOMO: -7.59742 LUMO: 0.00272 factor:1 | -1 (0.79936) | 1 | 1 |
| G: -5313.11806 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.87164 HOMO: -6.99333 LUMO: -1.33880 factor:1 | -1 (0.61212) | -1 | -1 |
| G: -5313.11806 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.73591 HOMO: -6.63958 LUMO: -1.39322 factor:1 | -1 (0.74785) | -1 | -1 |
| G: -5313.11806 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.89139 HOMO: -7.86137 LUMO: 0.01633 factor:1 | -1 (0.59236) | 1 | 1 |
| G: -5313.11806 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.15583 HOMO: -7.29537 LUMO: 0.14694 factor:1 | -1 (0.32792) | 1 | 1 |
| G: -5313.11806 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.85346 HOMO: -6.95523 LUMO: 0.48708 factor:1 | -1 (0.63030) | -1 | -1 |
| G: -5313.11806 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.84862 HOMO: -7.10217 LUMO: -1.10478 factor:1 | -1 (0.63514) | 1 | 1 |
| G: -5313.11806 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.71857 HOMO: -6.88176 LUMO: -0.96328 factor:1 | -1 (0.76518) | -1 | -1 |
| G: -5313.11806 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.41503 HOMO: -7.89130 LUMO: -0.13334 factor:1 | -1 (1.06873) | 1 | 1 |
| G: -5313.11806 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.74089 HOMO: -7.75252 LUMO: 0.25579 factor:1 | -1 (0.74287) | 1 | 1 |
| G: -5313.11806 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.96562 HOMO: -6.87632 LUMO: -0.93063 factor:1 | -1 (0.51813) | -1 | -1 |
| G: -5313.11806 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.63555 HOMO: -6.78108 LUMO: -0.86804 factor:1 | -1 (0.84821) | -1 | -1 |
| G: -5313.11806 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.75743 HOMO: -5.98106 LUMO: 0.10340 factor:1 | -1 (0.72633) | -1 | -1 |
| G: -5313.11806 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.54842 HOMO: -6.40284 LUMO: -0.87349 factor:1 | -1 (0.93534) | -1 | -1 |
| G: -5313.11806 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.11017 HOMO: -6.77019 LUMO: -1.20819 factor:1 | -1 (0.37359) | -1 | -1 |
| G: -5313.11806 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.75640 HOMO: -6.90081 LUMO: -1.00682 factor:1 | -1 (0.72736) | -1 | -1 |
| G: -5313.11806 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.62377 HOMO: -6.59060 LUMO: -0.26667 factor:1 | -1 (0.85999) | -1 | -1 |
| G: -5313.11806 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.77509 HOMO: -6.50896 LUMO: -0.48708 factor:1 | -1 (0.70867) | -1 | -1 |
| G: -5313.11806 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.97354 HOMO: -6.20420 LUMO: -0.73471 factor:1 | -1 (0.51021) | -1 | -1 |
| G: -5313.11806 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.72023 HOMO: -6.17154 LUMO: -0.68573 factor:1 | -1 (0.76352) | -1 | -1 |
| G: -5313.11806 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.50423 HOMO: -6.21236 LUMO: 0.09796 factor:1 | -1 (0.97953) | -1 | -1 |
| G: -5313.11806 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.76668 HOMO: -6.38379 LUMO: 0.58232 factor:1 | -1 (0.71707) | -1 | -1 |
| G: -5313.11806 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.78328 HOMO: -7.42871 LUMO: 0.40273 factor:1 | -1 (0.70048) | 1 | 1 |
| G: -5313.11806 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.83596 HOMO: -6.54978 LUMO: 0.26395 factor:1 | -1 (0.64779) | -1 | -1 |
| G: -5313.11806 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.87879 HOMO: -7.14027 LUMO: 0.14150 factor:1 | -1 (0.60496) | 1 | 1 |
| G: -5313.11806 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.06726 HOMO: -7.25456 LUMO: -0.15783 factor:1 | -1 (0.41650) | 1 | 1 |
| G: -5313.11806 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.90992 HOMO: -6.90897 LUMO: 0.63403 factor:1 | -1 (0.57383) | -1 | -1 |
| G: -5313.11806 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.82649 HOMO: -6.49264 LUMO: 0.71022 factor:1 | -1 (0.65726) | -1 | -1 |
| G: -5313.11806 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.70554 HOMO: -6.56067 LUMO: -1.03947 factor:1 | -1 (0.77822) | -1 | -1 |
| G: -5313.11806 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.90200 HOMO: -6.79196 LUMO: -1.12655 factor:1 | -1 (0.58175) | -1 | -1 |
| G: -5313.11806 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.74407 HOMO: -6.95251 LUMO: -1.09118 factor:1 | -1 (0.73969) | -1 | -1 |
| G: -5313.11806 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.78516 HOMO: -7.47225 LUMO: -0.22041 factor:1 | -1 (0.69860) | 1 | 1 |
| G: -5313.11806 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.54807 HOMO: -7.13483 LUMO: -0.98505 factor:1 | -1 (0.93569) | 1 | 1 |
| G: -5313.11806 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.60782 HOMO: -6.99061 LUMO: -1.05852 factor:1 | -1 (0.87593) | -1 | -1 |
| G: -5313.11806 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.43008 HOMO: -6.52257 LUMO: -1.11022 factor:1 | -1 (1.05368) | -1 | -1 |
| G: -5313.11806 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.74780 HOMO: -6.75114 LUMO: -1.09934 factor:1 | -1 (0.73596) | -1 | -1 |
| G: -5313.11806 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.09861 HOMO: -6.82189 LUMO: -0.89253 factor:1 | -1 (0.38515) | -1 | -1 |
| G: -5313.11806 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.96581 HOMO: -6.83278 LUMO: -0.97961 factor:1 | -1 (0.51794) | -1 | -1 |
| G: -5313.11806 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.06669 HOMO: -6.65318 LUMO: -0.84355 factor:1 | -1 (0.41707) | -1 | -1 |
| G: -5313.11806 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.95052 HOMO: -6.75931 LUMO: -0.88437 factor:1 | -1 (0.53323) | -1 | -1 |
| G: -5313.11806 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.89381 HOMO: -6.19059 LUMO: -0.45715 factor:1 | -1 (0.58994) | -1 | -1 |
| G: -5313.11806 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.75468 HOMO: -7.09673 LUMO: -2.01908 factor:1 | -1 (0.72907) | -1 | -1 |
| G: -5313.11806 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.78323 HOMO: -7.88042 LUMO: 0.38640 factor:1 | -1 (0.70053) | 1 | 1 |
| G: -5313.11806 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.71925 HOMO: -7.83144 LUMO: 0.14422 factor:1 | -1 (0.76450) | 1 | 1 |
| G: -5313.11806 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.99975 HOMO: -7.46408 LUMO: 0.44627 factor:1 | -1 (0.48401) | 1 | 1 |
| G: -5313.11806 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.68366 HOMO: -7.12394 LUMO: -2.04902 factor:1 | -1 (0.80010) | -1 | -1 |
| G: -5313.11806 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.91482 HOMO: -6.78380 LUMO: -1.11295 factor:1 | -1 (0.56894) | -1 | -1 |
| G: -5313.11806 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.63188 HOMO: -7.12938 LUMO: -0.23674 factor:1 | -1 (0.85188) | 1 | 1 |
| G: -5313.11806 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.78793 HOMO: -6.14705 LUMO: -0.20409 factor:1 | -1 (0.69582) | -1 | -1 |
| G: -5313.11806 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.48265 HOMO: -6.50080 LUMO: -0.28300 factor:1 | -1 (1.00111) | -1 | -1 |
| G: -5313.11806 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.77427 HOMO: -6.50352 LUMO: -0.62042 factor:1 | -1 (0.70948) | -1 | -1 |
| G: -5313.11806 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.60766 HOMO: -6.46543 LUMO: -0.53879 factor:1 | -1 (0.87610) | -1 | -1 |
| G: -5313.11806 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.65694 HOMO: -7.32803 LUMO: -0.52790 factor:1 | -1 (0.82682) | 1 | 1 |
| G: -5313.11806 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.39843 HOMO: -5.94025 LUMO: -0.17687 factor:1 | -1 (1.08533) | -1 | -1 |
| G: -5313.11806 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.97479 HOMO: -5.62187 LUMO: 0.05714 factor:1 | -1 (0.50896) | -1 | -1 |
| G: -5313.11806 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.03743 HOMO: -7.03414 LUMO: -1.04492 factor:1 | -1 (0.44632) | -1 | -1 |
| G: -5313.11806 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.13760 HOMO: -6.75387 LUMO: -2.02181 factor:1 | -1 (0.34616) | -1 | -1 |
| G: -5313.11806 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.09050 HOMO: -6.55250 LUMO: -0.75648 factor:1 | -1 (0.39326) | -1 | -1 |
| G: -5313.11806 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.11341 HOMO: -6.81101 LUMO: -1.02043 factor:1 | -1 (0.37035) | -1 | -1 |
| G: -5313.11806 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.85264 HOMO: -6.69672 LUMO: -2.81910 factor:1 | -1 (0.63111) | -1 | -1 |
| G: -5313.11806 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.86195 HOMO: -6.69128 LUMO: -2.58236 factor:1 | -1 (0.62181) | -1 | -1 |
| G: -5313.11806 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.26843 HOMO: -6.73482 LUMO: -2.06807 factor:1 | -1 (0.21532) | -1 | -1 |
| G: -5313.11806 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.09311 HOMO: -7.66545 LUMO: 0.17143 factor:1 | -1 (0.39065) | 1 | 1 |
| G: -5313.11806 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.16642 HOMO: -6.87904 LUMO: -1.25172 factor:1 | -1 (0.31734) | -1 | -1 |
| G: -5313.11806 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.03765 HOMO: -6.84366 LUMO: -0.19320 factor:1 | -1 (0.44610) | -1 | -1 |
| G: -5313.11806 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.96701 HOMO: -6.97972 LUMO: -0.97961 factor:1 | -1 (0.51674) | -1 | -1 |
| G: -5313.11806 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.95469 HOMO: -6.72121 LUMO: -0.70477 factor:1 | -1 (0.52907) | -1 | -1 |
| G: -5313.11806 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.96048 HOMO: -7.18925 LUMO: 0.40001 factor:1 | -1 (0.52327) | 1 | 1 |
| G: -5313.11806 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.07602 HOMO: -6.72121 LUMO: 0.19592 factor:1 | -1 (0.40774) | -1 | -1 |
| G: -5313.11806 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.20103 HOMO: -6.85999 LUMO: -0.39457 factor:1 | -1 (0.28273) | -1 | -1 |
| G: -5313.11806 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.24808 HOMO: -6.90625 LUMO: 0.05987 factor:1 | -1 (0.23568) | -1 | -1 |
| G: -5313.11806 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.09031 HOMO: -7.00421 LUMO: 0.37552 factor:1 | -1 (0.39345) | -1 | -1 |
| G: -5313.11806 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.04266 HOMO: -6.56883 LUMO: -0.97689 factor:1 | -1 (0.44110) | -1 | -1 |
| G: -5313.11806 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.75539 HOMO: -6.66679 LUMO: 0.56055 factor:1 | -1 (0.72837) | -1 | -1 |
| G: -5313.11806 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.75144 HOMO: -6.75931 LUMO: 0.32926 factor:1 | -1 (0.73231) | -1 | -1 |
| G: -5313.11806 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.83623 HOMO: -6.53617 LUMO: -1.06397 factor:1 | -1 (0.64752) | -1 | -1 |
| G: -5313.11806 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.10974 HOMO: -6.78108 LUMO: 0.42722 factor:1 | -1 (0.37402) | -1 | -1 |
| G: -5313.11806 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.86965 HOMO: -7.05319 LUMO: 0.61498 factor:1 | -1 (0.61411) | -1 | -1 |
| G: -5313.11806 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.16359 HOMO: -6.78380 LUMO: 1.49391 factor:1 | -1 (0.32017) | -1 | -1 |
| G: -5313.11806 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.74208 HOMO: -7.21102 LUMO: 0.27211 factor:1 | -1 (0.74167) | 1 | 1 |
| G: -5313.11806 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.93556 HOMO: -6.67223 LUMO: 0.81362 factor:1 | -1 (0.54820) | -1 | -1 |
| G: -5313.11806 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.76067 HOMO: -6.69944 LUMO: 1.40683 factor:1 | -1 (0.72309) | -1 | -1 |
| G: -5313.11806 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.54066 HOMO: -7.02598 LUMO: 1.46941 factor:1 | -1 (0.94309) | -1 | -1 |
| G: -5313.11806 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.68371 HOMO: -5.85045 LUMO: -0.76736 factor:1 | -1 (0.80004) | -1 | -1 |
| G: -5313.11806 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.86832 HOMO: -6.53890 LUMO: -0.50885 factor:1 | -1 (0.61544) | -1 | -1 |
| G: -5313.11806 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.85022 HOMO: -6.42733 LUMO: -0.63947 factor:1 | -1 (0.63354) | -1 | -1 |
| G: -5313.11806 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.12492 HOMO: -6.82189 LUMO: -0.85444 factor:1 | -1 (0.35884) | -1 | -1 |
| G: -5313.11806 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.86192 HOMO: -6.97428 LUMO: -1.22179 factor:1 | -1 (0.62183) | -1 | -1 |
| G: -5313.11806 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.96160 HOMO: -6.93346 LUMO: -1.09934 factor:1 | -1 (0.52216) | -1 | -1 |
| G: -5313.11806 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.74148 HOMO: -7.17292 LUMO: -1.11839 factor:1 | -1 (0.74227) | 1 | 1 |
| G: -5313.11806 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.05752 HOMO: -7.00965 LUMO: -1.23268 factor:1 | -1 (0.42624) | -1 | -1 |
| G: -5313.11806 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.20187 HOMO: -6.73210 LUMO: -1.12383 factor:1 | -1 (0.28188) | -1 | -1 |
| G: -5313.11806 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.82102 HOMO: -7.61375 LUMO: -0.11973 factor:1 | -1 (0.66273) | 1 | 1 |
| G: -5313.11806 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.64412 HOMO: -7.42327 LUMO: 0.41906 factor:1 | -1 (0.83963) | 1 | 1 |
| G: -5313.11806 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.94372 HOMO: -6.94162 LUMO: -1.01771 factor:1 | -1 (0.54004) | -1 | -1 |
| G: -5313.11806 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.71166 HOMO: -6.82189 LUMO: -0.92791 factor:1 | -1 (0.77210) | -1 | -1 |
| G: -5313.11806 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.63095 HOMO: -6.92258 LUMO: -1.73881 factor:1 | -1 (0.85280) | -1 | -1 |
| G: -5313.11806 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.45688 HOMO: -6.50896 LUMO: -1.60819 factor:1 | -1 (1.02688) | -1 | -1 |
| G: -5313.11806 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.96328 HOMO: -6.38379 LUMO: -2.18780 factor:1 | -1 (0.52047) | -1 | -1 |
| G: -5313.11806 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.91428 HOMO: -6.48992 LUMO: -0.97417 factor:1 | -1 (0.56948) | -1 | -1 |
| G: -5313.11806 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.16329 HOMO: -6.01644 LUMO: -0.04354 factor:1 | -1 (0.32047) | -1 | -1 |
| G: -5313.11806 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.81452 HOMO: -6.70761 LUMO: -0.14422 factor:1 | -1 (0.66924) | -1 | -1 |
| G: -5313.11806 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.68905 HOMO: -6.70216 LUMO: 0.14422 factor:1 | -1 (0.79471) | -1 | -1 |
| G: -5313.11806 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.73563 HOMO: -7.07224 LUMO: -0.10885 factor:1 | -1 (0.74812) | 1 | 1 |
| G: -5313.11806 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.96845 HOMO: -7.52667 LUMO: -0.74287 factor:1 | -1 (0.51530) | 1 | 1 |
| G: -5313.11806 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.71142 HOMO: -6.48447 LUMO: -0.96056 factor:1 | -1 (0.77234) | -1 | -1 |
| G: -5313.11806 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.72592 HOMO: -6.22597 LUMO: -0.41361 factor:1 | -1 (0.75784) | -1 | -1 |
| G: -5313.11806 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.52129 HOMO: -6.12256 LUMO: -1.05852 factor:1 | -1 (0.96247) | -1 | -1 |
| G: -5313.11806 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.59177 HOMO: -6.97428 LUMO: -0.60681 factor:1 | -1 (0.89199) | -1 | -1 |
| G: -5313.11806 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.54140 HOMO: -6.78380 LUMO: -0.88981 factor:1 | -1 (0.94236) | -1 | -1 |
| G: -5313.11806 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.32188 HOMO: -6.85999 LUMO: 0.07891 factor:1 | -1 (1.16187) | -1 | -1 |
| G: -5313.11806 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.75631 HOMO: -7.08312 LUMO: -0.60137 factor:1 | -1 (0.72744) | 1 | 1 |
| G: -5313.11806 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.63870 HOMO: -6.57699 LUMO: -0.68028 factor:1 | 1 (-0.15494) | -1 | -1 |
| G: -5313.11806 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.80153 HOMO: -6.09807 LUMO: -0.31837 factor:1 | 1 (-0.31777) | -1 | -1 |
| G: -5313.11806 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.67432 HOMO: -6.10624 LUMO: 0.14966 factor:1 | 1 (-0.19056) | -1 | -1 |
| G: -5313.11806 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.73644 HOMO: -6.77019 LUMO: -0.95784 factor:1 | 1 (-0.25268) | -1 | -1 |
| G: -5313.11806 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.96877 HOMO: -5.93208 LUMO: -0.44627 factor:1 | 1 (-0.48502) | -1 | -1 |
| G: -5313.11806 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.95876 HOMO: -6.12256 LUMO: -0.27756 factor:1 | 1 (-0.47500) | -1 | -1 |
| G: -5313.11806 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.90872 HOMO: -5.98106 LUMO: -0.37824 factor:1 | 1 (-0.42496) | -1 | -1 |
| G: -5313.11806 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.92774 HOMO: -7.06408 LUMO: -1.12927 factor:1 | 1 (-0.44398) | 1 | 1 |
| G: -5313.11806 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.65769 HOMO: -6.70761 LUMO: -0.98505 factor:1 | 1 (-0.17394) | -1 | -1 |
| G: -5313.11806 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.63043 HOMO: -7.00965 LUMO: -0.42722 factor:1 | 1 (-0.14667) | -1 | -1 |
| G: -5313.11806 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.45026 HOMO: -5.96201 LUMO: -0.59049 factor:1 | -1 (0.03350) | -1 | -1 |
| G: -5313.11806 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.56498 HOMO: -6.34570 LUMO: -1.68438 factor:1 | 1 (-0.08123) | -1 | -1 |
| G: -5313.11806 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.49097 HOMO: -6.97156 LUMO: -1.85854 factor:1 | 1 (-0.00721) | -1 | -1 |
| G: -5313.11806 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.48065 HOMO: -5.91848 LUMO: -2.51433 factor:1 | -1 (0.00310) | -1 | -1 |
| G: -5313.11806 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.65290 HOMO: -6.39195 LUMO: -1.66262 factor:1 | 1 (-0.16915) | -1 | -1 |
| G: -5313.11806 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.98152 HOMO: -6.50352 LUMO: 0.19592 factor:1 | -1 (0.50224) | -1 | -1 |
| G: -5313.11806 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.05708 HOMO: -6.45998 LUMO: 0.34831 factor:1 | -1 (0.42667) | -1 | -1 |
| G: -5313.11806 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.11439 HOMO: -7.05319 LUMO: 0.23402 factor:1 | -1 (0.36937) | -1 | -1 |
| G: -5313.11806 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.17559 HOMO: -6.61237 LUMO: 0.18232 factor:1 | -1 (0.30817) | -1 | -1 |
| G: -5313.11806 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.18280 HOMO: -6.57427 LUMO: 0.40545 factor:1 | -1 (0.30096) | -1 | -1 |
| G: -5313.11806 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.11270 HOMO: -7.26544 LUMO: 0.41089 factor:1 | -1 (0.37105) | 1 | 1 |
| G: -5313.11806 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.90410 HOMO: -6.26406 LUMO: -0.85444 factor:1 | -1 (0.57966) | -1 | -1 |
| G: -5313.11806 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.87038 HOMO: -6.25318 LUMO: -0.79457 factor:1 | -1 (0.61337) | -1 | -1 |
| G: -5313.11806 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.75283 HOMO: -6.68040 LUMO: 0.41089 factor:1 | -1 (0.73093) | -1 | -1 |
| G: -5313.11806 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.90707 HOMO: -6.37835 LUMO: 0.37280 factor:1 | -1 (0.57669) | -1 | -1 |
| G: -5313.11806 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.67103 HOMO: -6.56067 LUMO: 0.62858 factor:1 | -1 (0.81272) | -1 | -1 |
| G: -5313.11806 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.89659 HOMO: -6.74026 LUMO: -0.04082 factor:1 | -1 (0.58717) | -1 | -1 |
| G: -5313.11806 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.69893 HOMO: -6.53617 LUMO: 0.35103 factor:1 | -1 (0.78483) | -1 | -1 |
| G: -5313.11806 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.93077 HOMO: -6.51985 LUMO: 0.25851 factor:1 | -1 (0.55299) | -1 | -1 |
| G: -5313.11806 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.89904 HOMO: -6.58788 LUMO: -1.98371 factor:1 | -1 (0.58472) | -1 | -1 |
| G: -5313.11806 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.77642 HOMO: -6.51441 LUMO: 0.29116 factor:1 | -1 (0.70733) | -1 | -1 |
| G: -5313.11806 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.86100 HOMO: -6.81101 LUMO: 0.35647 factor:1 | -1 (0.62276) | -1 | -1 |
| G: -5313.11806 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.59930 HOMO: -6.42733 LUMO: 0.10340 factor:1 | -1 (0.88445) | -1 | -1 |
| G: -5313.11806 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.92663 HOMO: -6.70761 LUMO: 0.28028 factor:1 | -1 (0.55713) | -1 | -1 |
| G: -5313.11806 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.68611 HOMO: -6.67495 LUMO: 0.01633 factor:1 | -1 (0.79765) | -1 | -1 |
| G: -5313.11806 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.55683 HOMO: -6.75387 LUMO: 0.15510 factor:1 | -1 (0.92693) | -1 | -1 |
| G: -5313.11806 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.51397 HOMO: -6.56067 LUMO: 0.35919 factor:1 | -1 (0.96979) | -1 | -1 |
| G: -5313.11806 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.76355 HOMO: -7.16748 LUMO: 0.21497 factor:1 | -1 (0.72020) | 1 | 1 |
| G: -5313.11806 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.57638 HOMO: -6.71849 LUMO: 0.26667 factor:1 | 1 (-0.09263) | -1 | -1 |
| G: -5313.11806 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.40958 HOMO: -6.69128 LUMO: 0.55783 factor:1 | -1 (0.07418) | -1 | -1 |
| G: -5313.11806 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.54188 HOMO: -6.71305 LUMO: 0.45987 factor:1 | 1 (-0.05812) | -1 | -1 |
| G: -5313.11806 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.58384 HOMO: -5.90487 LUMO: -0.70750 factor:1 | 1 (-0.10008) | -1 | -1 |
| G: -5313.11806 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.70945 HOMO: -6.84638 LUMO: -0.72110 factor:1 | 1 (-0.22569) | -1 | -1 |
| G: -5313.11806 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.77786 HOMO: -6.66135 LUMO: -1.13471 factor:1 | 1 (-0.29410) | -1 | -1 |
| G: -5313.11806 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.55861 HOMO: -6.74026 LUMO: -0.64763 factor:1 | 1 (-0.07486) | -1 | -1 |
| G: -5313.11806 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.61418 HOMO: -6.69672 LUMO: -1.05036 factor:1 | 1 (-0.13042) | -1 | -1 |
| G: -5313.11806 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.50438 HOMO: -6.78924 LUMO: -1.03675 factor:1 | 1 (-0.02063) | -1 | -1 |
| G: -5313.11806 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.91176 HOMO: -6.81373 LUMO: -0.85988 factor:1 | 1 (-0.42801) | -1 | -1 |
| G: -5313.11806 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.48765 HOMO: -7.26544 LUMO: 0.91158 factor:1 | 1 (-0.00389) | 1 | 1 |
| G: -5313.11806 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.36862 HOMO: -6.64230 LUMO: -1.92929 factor:1 | -1 (0.11513) | -1 | -1 |
| G: -5313.11806 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.25153 HOMO: -7.20830 LUMO: 0.11429 factor:1 | -1 (0.23222) | 1 | 1 |
| G: -5313.11806 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.34509 HOMO: -7.17020 LUMO: 0.04898 factor:1 | -1 (0.13867) | 1 | 1 |
| G: -5313.11806 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.64632 HOMO: -7.16476 LUMO: 0.04898 factor:1 | 1 (-0.16256) | 1 | 1 |
| G: -5313.11806 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.79182 HOMO: -6.59332 LUMO: -0.49253 factor:1 | 1 (-0.30806) | -1 | -1 |
| G: -5313.11806 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.57162 HOMO: -7.46953 LUMO: 0.84083 factor:1 | 1 (-0.08787) | 1 | 1 |
| G: -5313.11806 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.62871 HOMO: -7.39878 LUMO: 0.88709 factor:1 | 1 (-0.14496) | 1 | 1 |
| G: -5313.11806 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.87715 HOMO: -6.84094 LUMO: -0.61498 factor:1 | 1 (-0.39340) | -1 | -1 |
| G: -5313.11806 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.87813 HOMO: -6.03549 LUMO: -0.27211 factor:1 | 1 (-0.39437) | -1 | -1 |
| G: -5313.11806 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.57652 HOMO: -7.31170 LUMO: -0.64763 factor:1 | 1 (-0.09276) | 1 | 1 |
| G: -5313.11806 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.59940 HOMO: -6.88992 LUMO: -0.84627 factor:1 | 1 (-0.11565) | -1 | -1 |
| G: -5313.11806 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.48025 HOMO: -7.12666 LUMO: -0.09252 factor:1 | -1 (0.00351) | 1 | 1 |
| G: -5313.11806 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.39891 HOMO: -6.70489 LUMO: -0.63675 factor:1 | -1 (0.08485) | -1 | -1 |
| G: -5313.11806 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.41015 HOMO: -6.98788 LUMO: 0.86804 factor:1 | -1 (0.07361) | -1 | -1 |
| G: -5313.11806 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.72392 HOMO: -6.80285 LUMO: -0.60954 factor:1 | 1 (-0.24017) | -1 | -1 |
| G: -5313.11806 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.55203 HOMO: -7.02054 LUMO: -0.74287 factor:1 | 1 (-0.06827) | -1 | -1 |
| G: -5313.11806 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.55497 HOMO: -7.03686 LUMO: -0.81090 factor:1 | 1 (-0.07121) | -1 | -1 |
| G: -5313.11806 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11578.15727 HOMO: -6.70489 LUMO: -1.00954 factor:1 | 1 (-0.67351) | -1 | -1 |
| G: -5313.11806 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11578.38769 HOMO: -7.69810 LUMO: 0.00544 factor:1 | 1 (-0.90394) | 1 | 1 |
| G: -5313.11806 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11578.98297 HOMO: -6.83550 LUMO: -0.11157 factor:1 | 1 (-1.49921) | -1 | -1 |
| G: -5313.11806 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.97255 HOMO: -6.76203 LUMO: -2.13609 factor:1 | 1 (-0.48880) | -1 | -1 |
| G: -5313.11806 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.96265 HOMO: -6.72121 LUMO: -2.62862 factor:1 | 1 (-0.47889) | -1 | -1 |
| G: -5313.11806 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11578.18861 HOMO: -6.48719 LUMO: -2.73474 factor:1 | 1 (-0.70486) | -1 | -1 |
| G: -5313.11806 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.99873 HOMO: -6.83006 LUMO: -0.00544 factor:1 | 1 (-0.51498) | -1 | -1 |
| G: -5313.11806 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.96820 HOMO: -6.84094 LUMO: -1.11022 factor:1 | 1 (-0.48444) | -1 | -1 |
| G: -5313.11806 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11578.19425 HOMO: -6.66951 LUMO: -1.23812 factor:1 | 1 (-0.71049) | -1 | -1 |
| G: -5313.11806 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.83141 HOMO: -6.78380 LUMO: -1.27894 factor:1 | 1 (-0.34765) | -1 | -1 |
| G: -5313.11806 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11578.98033 HOMO: -6.50352 LUMO: -0.56055 factor:1 | 1 (-1.49657) | -1 | -1 |
| G: -5313.11806 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11578.98218 HOMO: -7.77974 LUMO: -0.26395 factor:1 | 1 (-1.49842) | 1 | 1 |
| G: -5313.11806 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.79497 HOMO: -7.01510 LUMO: -1.64085 factor:1 | 1 (-0.31122) | -1 | -1 |
| G: -5313.11806 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11578.00496 HOMO: -6.59876 LUMO: -0.91158 factor:1 | 1 (-0.52121) | -1 | -1 |
| G: -5313.11806 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.93108 HOMO: -4.67219 LUMO: -0.67756 factor:1 | 1 (-0.44733) | -1 | -1 |
| G: -5313.11806 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.82882 HOMO: -6.70489 LUMO: -0.65579 factor:1 | 1 (-0.34507) | -1 | -1 |
| G: -5313.11806 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.58974 HOMO: -6.62325 LUMO: -0.60409 factor:1 | 1 (-0.10599) | -1 | -1 |
| G: -5313.11806 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11578.11101 HOMO: -6.20147 LUMO: 0.15238 factor:1 | 1 (-0.62725) | -1 | -1 |
| G: -5313.11806 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11578.38206 HOMO: -6.43549 LUMO: -0.07075 factor:1 | 1 (-0.89830) | -1 | -1 |
| G: -5313.11806 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11578.12611 HOMO: -7.02054 LUMO: 0.13061 factor:1 | 1 (-0.64235) | -1 | -1 |
| G: -5313.11806 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11578.10246 HOMO: -7.04503 LUMO: 0.30749 factor:1 | 1 (-0.61871) | -1 | -1 |
| G: -5313.11806 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.89930 HOMO: -6.74842 LUMO: -0.99594 factor:1 | 1 (-0.41555) | -1 | -1 |
| G: -5313.11806 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.80412 HOMO: -6.35658 LUMO: 0.41633 factor:1 | -1 (0.67963) | -1 | -1 |
| G: -5313.11806 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.83515 HOMO: -6.79740 LUMO: 0.56872 factor:1 | -1 (0.64861) | -1 | -1 |
| G: -5313.11806 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.02075 HOMO: -6.51713 LUMO: -0.05987 factor:1 | -1 (0.46300) | -1 | -1 |
| G: -5313.11806 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.78886 HOMO: -6.68040 LUMO: 0.34558 factor:1 | -1 (0.69490) | -1 | -1 |
| G: -5313.11806 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.73950 HOMO: -6.39740 LUMO: 0.50069 factor:1 | -1 (0.74426) | -1 | -1 |
| G: -5313.11806 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.80244 HOMO: -6.91713 LUMO: -0.97145 factor:1 | -1 (0.68132) | -1 | -1 |
| G: -5313.11806 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.59253 HOMO: -7.10761 LUMO: -0.27483 factor:1 | -1 (0.89123) | 1 | -1 |
| G: -5313.11806 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.69710 HOMO: -6.98788 LUMO: 0.40273 factor:1 | -1 (0.78665) | -1 | -1 |
| G: -5313.11806 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.88628 HOMO: -6.87087 LUMO: 0.28572 factor:1 | -1 (0.59748) | -1 | -1 |
| G: -5313.11806 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.77851 HOMO: -7.36612 LUMO: -0.12245 factor:1 | 1 (-0.29475) | 1 | 1 |
| G: -5313.11806 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11578.60606 HOMO: -6.72938 LUMO: 0.33742 factor:1 | 1 (-1.12231) | -1 | -1 |
| G: -5313.11806 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.94219 HOMO: -7.32531 LUMO: 0.07619 factor:1 | 1 (-0.45843) | 1 | 1 |
| G: -5313.11806 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.83549 HOMO: -6.87087 LUMO: -0.08436 factor:1 | 1 (-0.35173) | -1 | -1 |
| G: -5313.11806 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.77712 HOMO: -6.67495 LUMO: 0.85988 factor:1 | 1 (-0.29337) | -1 | -1 |
| G: -5313.11806 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.57110 HOMO: -6.96339 LUMO: 0.65307 factor:1 | 1 (-0.08735) | -1 | -1 |
| G: -5313.11806 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.80442 HOMO: -6.58516 LUMO: -0.78641 factor:1 | 1 (-0.32066) | -1 | -1 |
| G: -5313.11806 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.61530 HOMO: -6.56883 LUMO: 0.44355 factor:1 | 1 (-0.13154) | -1 | -1 |
| G: -5313.11806 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.80771 HOMO: -6.68312 LUMO: 0.43538 factor:1 | 1 (-0.32395) | -1 | -1 |
| G: -5313.11806 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.65108 HOMO: -6.81917 LUMO: 0.20681 factor:1 | 1 (-0.16732) | -1 | -1 |
| G: -5313.11806 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.80096 HOMO: -6.91169 LUMO: 0.08163 factor:1 | 1 (-0.31720) | -1 | -1 |
| G: -5313.11806 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.76194 HOMO: -4.88444 LUMO: -0.49253 factor:1 | 1 (-0.27818) | -1 | -1 |
| G: -5313.11806 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.88070 HOMO: -6.42189 LUMO: 0.64763 factor:1 | -1 (0.60306) | -1 | -1 |
| G: -5313.11806 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.90424 HOMO: -6.24501 LUMO: 0.55783 factor:1 | -1 (0.57952) | -1 | -1 |
| G: -5313.11806 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.00598 HOMO: -6.41372 LUMO: 0.29388 factor:1 | -1 (0.47778) | -1 | -1 |
| G: -5313.11806 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.12816 HOMO: -5.67902 LUMO: 1.77690 factor:1 | -1 (0.35560) | -1 | -1 |
| G: -5313.11806 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.02026 HOMO: -6.55794 LUMO: 0.05170 factor:1 | -1 (0.46349) | -1 | -1 |
| G: -5313.11806 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.92772 HOMO: -6.52801 LUMO: 0.25851 factor:1 | -1 (0.55604) | -1 | -1 |
| G: -5313.11806 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.90870 HOMO: -7.08857 LUMO: 0.11157 factor:1 | -1 (0.57506) | 1 | 1 |
| G: -5313.11806 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.04040 HOMO: -6.58243 LUMO: 0.75648 factor:1 | -1 (0.44336) | -1 | -1 |
| G: -5313.11806 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.96747 HOMO: -7.22190 LUMO: 0.45171 factor:1 | -1 (0.51628) | 1 | 1 |
| G: -5313.11806 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.68956 HOMO: -6.47087 LUMO: 0.00000 factor:1 | -1 (0.79419) | -1 | -1 |
| G: -5313.11806 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.93128 HOMO: -6.78652 LUMO: 1.32247 factor:1 | -1 (0.55247) | -1 | -1 |
| G: -5313.11806 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.76001 HOMO: -6.74026 LUMO: 1.45309 factor:1 | -1 (0.72374) | -1 | -1 |
| G: -5313.11806 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.96421 HOMO: -6.69944 LUMO: 0.76464 factor:1 | -1 (0.51955) | -1 | -1 |
| G: -5313.11806 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.01020 HOMO: -6.62325 LUMO: 0.64763 factor:1 | -1 (0.47356) | -1 | -1 |
| G: -5313.11806 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.77836 HOMO: -6.45182 LUMO: 0.49253 factor:1 | -1 (0.70540) | -1 | -1 |
| G: -5313.11806 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.00339 HOMO: -7.14843 LUMO: 0.62586 factor:1 | -1 (0.48036) | 1 | 1 |
| G: -5313.11806 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.81721 HOMO: -6.87087 LUMO: 1.53200 factor:1 | -1 (0.66654) | -1 | -1 |
| G: -5313.11806 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.98712 HOMO: -6.54978 LUMO: 0.45171 factor:1 | -1 (0.49664) | -1 | -1 |
| G: -5313.11806 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.77871 HOMO: -6.63686 LUMO: 0.80001 factor:1 | -1 (0.70505) | -1 | -1 |
| G: -5313.11806 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.09684 HOMO: -7.00693 LUMO: 1.56193 factor:1 | -1 (0.38692) | -1 | -1 |
| G: -5313.11806 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.80837 HOMO: -6.02460 LUMO: 1.72792 factor:1 | -1 (0.67539) | -1 | -1 |
| G: -5313.11806 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.56178 HOMO: -6.36746 LUMO: -1.20002 factor:1 | -1 (0.92198) | -1 | -1 |
| G: -5313.11806 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.81928 HOMO: -7.26816 LUMO: -1.06397 factor:1 | -1 (0.66447) | 1 | 1 |
| G: -5313.11806 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.04212 HOMO: -7.34707 LUMO: -1.09662 factor:1 | -1 (0.44164) | 1 | 1 |
| G: -5313.11806 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.84208 HOMO: -7.93212 LUMO: -0.13606 factor:1 | -1 (0.64167) | 1 | 1 |
| G: -5313.11806 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.93322 HOMO: -6.80285 LUMO: 0.58504 factor:1 | -1 (0.55054) | -1 | -1 |
| G: -5313.11806 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.72227 HOMO: -7.12938 LUMO: 0.32926 factor:1 | -1 (0.76148) | 1 | -1 |
| G: -5313.11806 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.04337 HOMO: -6.86815 LUMO: -1.30070 factor:1 | -1 (0.44039) | -1 | -1 |
| G: -5313.11806 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.83278 HOMO: -6.99333 LUMO: -1.03947 factor:1 | -1 (0.65098) | -1 | -1 |
| G: -5313.11806 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.79207 HOMO: -7.56749 LUMO: -0.11157 factor:1 | -1 (0.69169) | 1 | 1 |
| G: -5313.11806 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.51941 HOMO: -7.57293 LUMO: -0.07891 factor:1 | -1 (0.96434) | 1 | 1 |
| G: -5313.11806 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.88617 HOMO: -7.30626 LUMO: 0.27211 factor:1 | -1 (0.59759) | 1 | 1 |
| G: -5313.11806 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.62926 HOMO: -7.77974 LUMO: 0.27211 factor:1 | -1 (0.85449) | 1 | 1 |
| G: -5313.11806 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.44537 HOMO: -7.11578 LUMO: 0.19864 factor:1 | -1 (1.03839) | 1 | 1 |
| G: -5313.11806 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.64423 HOMO: -7.71171 LUMO: 0.57688 factor:1 | -1 (0.83953) | 1 | 1 |
| G: -5313.11806 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.80597 HOMO: -7.83688 LUMO: 0.37824 factor:1 | -1 (0.67778) | 1 | 1 |
| G: -5313.11806 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.78347 HOMO: -6.94979 LUMO: -1.66534 factor:1 | -1 (0.70029) | -1 | -1 |
| G: -5313.11806 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.83830 HOMO: -6.97156 LUMO: -1.13199 factor:1 | -1 (0.64545) | -1 | -1 |
| G: -5313.11806 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.88540 HOMO: -6.91441 LUMO: -1.08301 factor:1 | -1 (0.59835) | -1 | -1 |
| G: -5313.11806 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.79493 HOMO: -6.71849 LUMO: -0.74831 factor:1 | -1 (0.68883) | -1 | -1 |
| G: -5313.11806 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.75939 HOMO: -7.09401 LUMO: -1.77690 factor:1 | -1 (0.72437) | -1 | -1 |
| G: -5313.11806 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.79498 HOMO: -6.97156 LUMO: -1.45037 factor:1 | -1 (0.68877) | -1 | -1 |
| G: -5313.11806 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.94500 HOMO: -7.22462 LUMO: -1.11295 factor:1 | -1 (0.53876) | 1 | 1 |
| G: -5313.11806 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.10780 HOMO: -7.85321 LUMO: 0.16599 factor:1 | -1 (0.37595) | 1 | 1 |
| G: -5313.11806 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.96911 HOMO: -7.71987 LUMO: 0.55511 factor:1 | -1 (0.51465) | 1 | 1 |
| G: -5313.11806 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.01485 HOMO: -7.63551 LUMO: 0.14422 factor:1 | -1 (0.46891) | 1 | 1 |
| G: -5313.11806 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.94728 HOMO: -6.98788 LUMO: -0.80546 factor:1 | -1 (0.53647) | -1 | -1 |
| G: -5313.11806 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.91156 HOMO: -6.98788 LUMO: -1.16737 factor:1 | -1 (0.57220) | -1 | -1 |
| G: -5313.11806 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.79046 HOMO: -6.56611 LUMO: -1.60819 factor:1 | -1 (0.69329) | -1 | -1 |
| G: -5313.11806 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.98707 HOMO: -6.95251 LUMO: 0.66396 factor:1 | -1 (0.49669) | -1 | -1 |
| G: -5313.11806 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.87191 HOMO: -7.35252 LUMO: 0.49797 factor:1 | -1 (0.61185) | 1 | 1 |
| G: -5313.11806 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.15814 HOMO: -6.90897 LUMO: -0.81090 factor:1 | -1 (0.32561) | -1 | -1 |
| G: -5313.11806 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.97226 HOMO: -7.04503 LUMO: -1.08301 factor:1 | -1 (0.51149) | -1 | -1 |
| G: -5313.11806 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.93123 HOMO: -6.92530 LUMO: -1.29526 factor:1 | -1 (0.55253) | -1 | -1 |
| G: -5313.11806 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.89789 HOMO: -6.93074 LUMO: -1.25444 factor:1 | -1 (0.58586) | -1 | -1 |
| G: -5313.11806 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.04990 HOMO: -6.73482 LUMO: -0.62042 factor:1 | -1 (0.43386) | -1 | -1 |
| G: -5313.11806 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.78608 HOMO: -7.67633 LUMO: 0.59593 factor:1 | -1 (0.69767) | 1 | 1 |
| G: -5313.11806 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.96845 HOMO: -7.39061 LUMO: -0.19320 factor:1 | -1 (0.51530) | 1 | 1 |
| G: -5313.11806 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.77359 HOMO: -7.55388 LUMO: -0.20136 factor:1 | -1 (0.71016) | 1 | 1 |
| G: -5313.11806 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.96737 HOMO: -7.14027 LUMO: -0.99866 factor:1 | -1 (0.51639) | 1 | 1 |
| G: -5313.11806 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.77528 HOMO: -6.75931 LUMO: -0.73199 factor:1 | -1 (0.70848) | -1 | -1 |
| G: -5313.11806 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.98138 HOMO: -5.45044 LUMO: -0.18776 factor:1 | -1 (0.50238) | -1 | -1 |
| G: -5313.11806 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.81403 HOMO: -6.70761 LUMO: -0.84083 factor:1 | -1 (0.66973) | -1 | -1 |
| G: -5313.11806 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.43704 HOMO: -6.05453 LUMO: -1.06669 factor:1 | -1 (1.04671) | -1 | -1 |
| G: -5313.11806 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.65620 HOMO: -6.86815 LUMO: -0.98233 factor:1 | -1 (0.82755) | -1 | -1 |
| G: -5313.11806 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.51533 HOMO: -6.73210 LUMO: -0.95240 factor:1 | -1 (0.96843) | -1 | -1 |
| G: -5313.11806 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.85691 HOMO: -5.89671 LUMO: -1.05036 factor:1 | -1 (0.62684) | -1 | -1 |
| G: -5313.11806 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.58203 HOMO: -7.61102 LUMO: 0.33470 factor:1 | -1 (0.90173) | 1 | 1 |
| G: -5313.11806 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.54646 HOMO: -7.51034 LUMO: 0.23674 factor:1 | -1 (0.93730) | 1 | 1 |
| G: -5313.11806 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.38580 HOMO: -7.41510 LUMO: 0.62858 factor:1 | -1 (1.09795) | 1 | 1 |
| G: -5313.11806 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.73158 HOMO: -6.76203 LUMO: -1.72792 factor:1 | -1 (0.75218) | -1 | -1 |
| G: -5313.11806 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.91675 HOMO: -6.60420 LUMO: -0.45715 factor:1 | -1 (0.56700) | -1 | -1 |
| G: -5313.11806 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.91068 HOMO: -6.59060 LUMO: -0.58232 factor:1 | -1 (0.57307) | -1 | -1 |
| G: -5313.11806 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.89278 HOMO: -7.43687 LUMO: -0.76736 factor:1 | -1 (0.59098) | 1 | 1 |
| G: -5313.11806 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.01104 HOMO: -6.08719 LUMO: -0.48708 factor:1 | -1 (0.47272) | -1 | -1 |
| G: -5313.11806 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.03980 HOMO: -5.88854 LUMO: -0.05714 factor:1 | -1 (0.44395) | -1 | -1 |
| G: -5313.11806 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.92524 HOMO: -7.34435 LUMO: -0.71838 factor:1 | -1 (0.55851) | 1 | 1 |
| G: -5313.11806 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.88745 HOMO: -7.46408 LUMO: -0.63130 factor:1 | -1 (0.59631) | 1 | 1 |
| G: -5313.11806 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.84663 HOMO: -7.00965 LUMO: -1.24900 factor:1 | -1 (0.63713) | -1 | -1 |
| G: -5313.11806 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.82842 HOMO: -6.91169 LUMO: -0.88981 factor:1 | -1 (0.65533) | -1 | -1 |
| G: -5313.11806 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.72116 HOMO: -6.78652 LUMO: -0.82178 factor:1 | -1 (0.76260) | -1 | -1 |
| G: -5313.11806 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.69435 HOMO: -7.80423 LUMO: 0.87076 factor:1 | -1 (0.78940) | 1 | 1 |
| G: -5313.11806 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.71814 HOMO: -6.97700 LUMO: -1.00954 factor:1 | -1 (0.76562) | -1 | -1 |
| G: -5313.11806 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.92380 HOMO: -6.92530 LUMO: -0.88165 factor:1 | -1 (0.55996) | -1 | -1 |
| G: -5313.11806 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.67005 HOMO: -7.14571 LUMO: -1.04492 factor:1 | 1 (-0.18629) | 1 | 1 |
| G: -5313.11806 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.79258 HOMO: -7.49674 LUMO: 0.34558 factor:1 | 1 (-0.30882) | 1 | 1 |
| G: -5313.11806 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.86420 HOMO: -6.44094 LUMO: -1.20819 factor:1 | 1 (-0.38044) | -1 | -1 |
| G: -5313.11806 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.47829 HOMO: -6.47359 LUMO: -1.14016 factor:1 | -1 (0.00547) | -1 | -1 |
| G: -5313.11806 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.43505 HOMO: -6.61237 LUMO: -0.87076 factor:1 | -1 (0.04871) | -1 | -1 |
| G: -5313.11806 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.44961 HOMO: -6.73754 LUMO: -1.09662 factor:1 | -1 (0.03415) | -1 | -1 |
| G: -5313.11806 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.43265 HOMO: -6.97700 LUMO: 0.13061 factor:1 | -1 (0.05110) | -1 | -1 |
| G: -5313.11806 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.28158 HOMO: -6.82734 LUMO: 0.59865 factor:1 | -1 (0.20218) | -1 | -1 |
| G: -5313.11806 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.62134 HOMO: -6.86543 LUMO: -0.91430 factor:1 | 1 (-0.13758) | -1 | -1 |
| G: -5313.11806 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.47763 HOMO: -6.74298 LUMO: 0.28028 factor:1 | -1 (0.00612) | -1 | -1 |
| G: -5313.11806 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.59516 HOMO: -6.75387 LUMO: 0.19592 factor:1 | 1 (-0.11140) | -1 | -1 |
| G: -5313.11806 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11578.21272 HOMO: -7.05591 LUMO: 0.10612 factor:1 | 1 (-0.72897) | -1 | -1 |
| G: -5313.11806 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11578.00401 HOMO: -6.86543 LUMO: 0.49253 factor:1 | 1 (-0.52025) | -1 | -1 |
| G: -5313.11806 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11578.02303 HOMO: -6.11440 LUMO: -1.12655 factor:1 | 1 (-0.53928) | -1 | -1 |
| G: -5313.11806 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11578.83529 HOMO: -6.77291 LUMO: -1.02859 factor:1 | 1 (-1.35154) | -1 | -1 |
| G: -5313.11806 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11578.98079 HOMO: -6.54978 LUMO: 0.29116 factor:1 | 1 (-1.49703) | -1 | -1 |
| G: -5313.11806 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.97506 HOMO: -7.18108 LUMO: 0.00000 factor:1 | 1 (-0.49130) | 1 | 1 |
| G: -5313.11806 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11578.15620 HOMO: -6.86271 LUMO: -1.15376 factor:1 | 1 (-0.67245) | -1 | -1 |
| G: -5313.11806 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.79141 HOMO: -6.78108 LUMO: -1.22723 factor:1 | 1 (-0.30765) | -1 | -1 |
| G: -5313.11806 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11578.04156 HOMO: -6.40828 LUMO: 0.02449 factor:1 | 1 (-0.55781) | -1 | -1 |
| G: -5313.11806 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.78665 HOMO: -6.43821 LUMO: 0.09796 factor:1 | 1 (-0.30289) | -1 | -1 |
| G: -5313.11806 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.80286 HOMO: -6.99877 LUMO: 0.40545 factor:1 | 1 (-0.31911) | -1 | -1 |
| G: -5313.11806 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.73818 HOMO: -6.68856 LUMO: 0.19320 factor:1 | 1 (-0.25443) | -1 | -1 |
| G: -5313.11806 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.59813 HOMO: -7.11034 LUMO: 0.31293 factor:1 | 1 (-0.11437) | 1 | 1 |
| G: -5313.11806 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.75245 HOMO: -6.92530 LUMO: -0.85444 factor:1 | -1 (0.73131) | -1 | -1 |
| G: -5313.11806 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.96494 HOMO: -6.60148 LUMO: -0.59865 factor:1 | -1 (0.51881) | -1 | -1 |
| G: -5313.11806 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.84187 HOMO: -6.72938 LUMO: 0.30749 factor:1 | -1 (0.64189) | -1 | -1 |
| G: -5313.11806 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.90619 HOMO: -7.31170 LUMO: 0.06803 factor:1 | -1 (0.57756) | 1 | 1 |
| G: -5313.11806 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.92399 HOMO: -7.09129 LUMO: -0.04626 factor:1 | -1 (0.55977) | 1 | 1 |
| G: -5313.11806 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.91158 HOMO: -6.38379 LUMO: -0.76736 factor:1 | -1 (0.57217) | -1 | -1 |
| G: -5313.11806 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.82829 HOMO: -6.13617 LUMO: -0.63947 factor:1 | -1 (0.65547) | -1 | -1 |
| G: -5313.11806 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.77049 HOMO: -6.92258 LUMO: 0.37007 factor:1 | -1 (0.71326) | -1 | -1 |
| G: -5313.11806 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.73539 HOMO: -6.35930 LUMO: 0.41361 factor:1 | -1 (0.74837) | -1 | -1 |
| G: -5313.11806 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.56192 HOMO: -6.60420 LUMO: 0.26667 factor:1 | -1 (0.92184) | -1 | -1 |
| G: -5313.11806 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.92170 HOMO: -6.04909 LUMO: 1.82588 factor:1 | -1 (0.56205) | -1 | -1 |
| G: -5313.11806 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.75297 HOMO: -6.69672 LUMO: 1.72520 factor:1 | -1 (0.73079) | -1 | -1 |
| G: -5313.11806 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.69699 HOMO: -6.50080 LUMO: 0.29116 factor:1 | -1 (0.78676) | -1 | -1 |
| G: -5313.11806 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.98160 HOMO: -6.60692 LUMO: -0.43266 factor:1 | -1 (0.50216) | -1 | -1 |
| G: -5313.11806 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.72401 HOMO: -6.93890 LUMO: 0.39729 factor:1 | -1 (0.75974) | -1 | -1 |
| G: -5313.11806 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.75727 HOMO: -6.52801 LUMO: -0.47076 factor:1 | -1 (0.72649) | -1 | -1 |
| G: -5313.11806 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.85528 HOMO: -6.41100 LUMO: 0.30477 factor:1 | -1 (0.62847) | -1 | -1 |
| G: -5313.11806 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.76763 HOMO: -6.37291 LUMO: -0.80001 factor:1 | -1 (0.71612) | -1 | -1 |
| G: -5313.11806 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.92845 HOMO: -6.51985 LUMO: 1.44765 factor:1 | -1 (0.55530) | -1 | -1 |
| G: -5313.11806 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.62467 HOMO: -6.64774 LUMO: 0.04626 factor:1 | -1 (0.85909) | -1 | -1 |
| G: -5313.11806 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.77778 HOMO: -6.65863 LUMO: 0.29933 factor:1 | -1 (0.70597) | -1 | -1 |
| G: -5313.11806 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.50012 HOMO: -7.09673 LUMO: 0.28300 factor:1 | -1 (0.98364) | 1 | 1 |
| G: -5313.11806 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.82051 HOMO: -6.57155 LUMO: -1.11567 factor:1 | -1 (0.66325) | -1 | -1 |
| G: -5313.11806 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.71103 HOMO: -6.38379 LUMO: -0.60681 factor:1 | -1 (0.77272) | -1 | -1 |
| G: -5313.11806 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.78891 HOMO: -6.60148 LUMO: 0.18232 factor:1 | -1 (0.69484) | -1 | -1 |
| G: -5313.11806 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.69014 HOMO: -6.96067 LUMO: -0.52246 factor:1 | -1 (0.79362) | -1 | -1 |
| G: -5313.11806 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.82894 HOMO: -6.57427 LUMO: -0.84627 factor:1 | -1 (0.65481) | -1 | -1 |
| G: -5313.11806 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.67944 HOMO: -6.59332 LUMO: -0.98233 factor:1 | -1 (0.80431) | -1 | -1 |
| G: -5313.11806 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.68910 HOMO: -6.20692 LUMO: -0.27483 factor:1 | -1 (0.79465) | -1 | -1 |
| G: -5313.11806 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.54450 HOMO: -6.81373 LUMO: 0.74559 factor:1 | -1 (0.93926) | -1 | -1 |
| G: -5313.11806 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.59109 HOMO: -6.60420 LUMO: 0.54695 factor:1 | -1 (0.89267) | -1 | -1 |
| G: -5313.11806 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.88883 HOMO: -6.58788 LUMO: -0.31021 factor:1 | -1 (0.59492) | -1 | -1 |
| G: -5313.11806 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.73686 HOMO: -6.72938 LUMO: 0.64763 factor:1 | -1 (0.74690) | -1 | -1 |
| G: -5313.11806 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.79438 HOMO: -6.86815 LUMO: 0.32109 factor:1 | -1 (0.68937) | -1 | -1 |
| G: -5313.11806 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.79302 HOMO: -6.63141 LUMO: 0.18776 factor:1 | -1 (0.69073) | -1 | -1 |
| G: -5313.11806 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11578.18801 HOMO: -7.18653 LUMO: 0.09524 factor:1 | 1 (-0.70426) | 1 | 1 |
| G: -5313.11806 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11578.97167 HOMO: -6.83550 LUMO: 0.03537 factor:1 | 1 (-1.48792) | -1 | -1 |
| G: -5313.11806 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.98662 HOMO: -7.47769 LUMO: 0.40817 factor:1 | 1 (-0.50287) | 1 | 1 |
| G: -5313.11806 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11578.13373 HOMO: -6.57971 LUMO: -0.63675 factor:1 | 1 (-0.64997) | -1 | -1 |
| G: -5313.11806 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11578.14733 HOMO: -6.74842 LUMO: -0.16327 factor:1 | 1 (-0.66358) | -1 | -1 |
| G: -5313.11806 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11578.00404 HOMO: -7.07224 LUMO: 0.61770 factor:1 | 1 (-0.52028) | 1 | 1 |
| G: -5313.11806 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.68978 HOMO: -6.83006 LUMO: 0.54695 factor:1 | -1 (0.79397) | -1 | -1 |
| G: -5313.11806 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.74864 HOMO: -6.60148 LUMO: 1.23540 factor:1 | -1 (0.73512) | -1 | -1 |
| G: -5313.11806 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.75269 HOMO: -6.99061 LUMO: 0.41089 factor:1 | -1 (0.73106) | -1 | -1 |
| G: -5313.11806 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.55775 HOMO: -6.63686 LUMO: 0.85172 factor:1 | -1 (0.92600) | -1 | -1 |
| G: -5313.11806 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.61917 HOMO: -6.50624 LUMO: 0.12517 factor:1 | -1 (0.86459) | -1 | -1 |
| G: -5313.11806 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.43552 HOMO: -6.35658 LUMO: 0.36463 factor:1 | -1 (1.04824) | -1 | -1 |
| G: -5313.11806 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.42877 HOMO: -6.34570 LUMO: 0.65035 factor:1 | -1 (1.05499) | -1 | -1 |
| G: -5313.11806 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.81506 HOMO: -6.63141 LUMO: 1.25717 factor:1 | -1 (0.66869) | -1 | -1 |
| G: -5313.11806 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.65373 HOMO: -6.91441 LUMO: 1.32792 factor:1 | -1 (0.83003) | -1 | -1 |
| G: -5313.11806 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.64442 HOMO: -7.15387 LUMO: 0.64219 factor:1 | -1 (0.83934) | 1 | 1 |
| G: -5313.11806 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.74826 HOMO: -7.17836 LUMO: 0.60409 factor:1 | -1 (0.73550) | 1 | 1 |
| G: -5313.11806 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11578.46035 HOMO: -6.92258 LUMO: 0.49525 factor:1 | 1 (-0.97659) | -1 | -1 |
| G: -5313.11806 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.67075 HOMO: -6.31032 LUMO: 0.48708 factor:1 | 1 (-0.18700) | -1 | -1 |
| G: -5313.11806 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.71456 HOMO: -6.49808 LUMO: 0.31021 factor:1 | 1 (-0.23081) | -1 | -1 |
| G: -5313.11806 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.74607 HOMO: -6.48447 LUMO: 0.37552 factor:1 | 1 (-0.26232) | -1 | -1 |
| G: -5313.11806 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.74722 HOMO: -6.66135 LUMO: -1.08301 factor:1 | 1 (-0.26346) | -1 | -1 |
| G: -5313.11806 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.60368 HOMO: -6.33481 LUMO: -0.51974 factor:1 | 1 (-0.11992) | -1 | -1 |
| G: -5313.11806 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.80047 HOMO: -6.76475 LUMO: -0.15238 factor:1 | 1 (-0.31671) | -1 | -1 |
| G: -5311.84231 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.03352 HOMO: -6.93346 LUMO: -0.10885 factor:1 | 1 (-0.82551) | -1 | -1 |
| G: -5311.84231 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.84902 HOMO: -7.19741 LUMO: 0.73199 factor:1 | 1 (-0.64102) | 1 | 1 |
| G: -5311.84231 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.57944 HOMO: -6.82734 LUMO: 0.88437 factor:1 | 1 (-0.37144) | -1 | -1 |
| G: -5311.84231 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11578.44220 HOMO: -7.01237 LUMO: 0.02721 factor:1 | 1 (-2.23419) | -1 | -1 |
| G: -5311.84231 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11578.06807 HOMO: -6.39195 LUMO: 1.46941 factor:1 | 1 (-1.86006) | -1 | -1 |
| G: -5311.84231 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11579.01581 HOMO: -6.53890 LUMO: 1.32792 factor:1 | 1 (-2.80781) | -1 | -1 |
| G: -5311.84231 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11578.14426 HOMO: -6.82734 LUMO: 1.98099 factor:1 | 1 (-1.93625) | -1 | -1 |
| G: -5311.84231 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11578.29803 HOMO: -6.74570 LUMO: 1.68983 factor:1 | 1 (-2.09002) | -1 | -1 |
| G: -5311.84231 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.87095 HOMO: -6.41100 LUMO: 1.39050 factor:1 | 1 (-1.66294) | -1 | -1 |
| G: -5311.84231 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.91870 HOMO: -5.92664 LUMO: 1.65989 factor:1 | 1 (-1.71070) | -1 | -1 |
| G: -5311.84231 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.90734 HOMO: -6.07630 LUMO: 1.54833 factor:1 | 1 (-0.69933) | -1 | -1 |
| G: -5311.84231 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.31279 HOMO: -6.45998 LUMO: 0.68573 factor:1 | 1 (-1.10478) | -1 | -1 |
| G: -5311.84231 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.94470 HOMO: -6.52801 LUMO: 0.41361 factor:1 | 1 (-0.73669) | -1 | -1 |
| G: -5311.84231 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.26729 HOMO: -6.77564 LUMO: 0.42178 factor:1 | 1 (-1.05928) | -1 | -1 |
| G: -5311.84231 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.20982 HOMO: -6.56339 LUMO: 1.65717 factor:1 | 1 (-1.00181) | -1 | -1 |
| G: -5311.84231 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.44933 HOMO: -5.85861 LUMO: 1.90752 factor:1 | 1 (-1.24133) | -1 | -1 |
| G: -5311.84231 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.61638 HOMO: -6.77019 LUMO: -2.48440 factor:1 | 1 (-1.40838) | -1 | -1 |
| G: -5311.84231 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.80545 HOMO: -6.53890 LUMO: -1.82588 factor:1 | 1 (-1.59744) | -1 | -1 |
| G: -5311.84231 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.94529 HOMO: -6.50352 LUMO: -1.66806 factor:1 | 1 (-1.73728) | -1 | -1 |
| G: -5311.84231 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.65973 HOMO: -6.90625 LUMO: 0.43538 factor:1 | 1 (-1.45173) | -1 | -1 |
| G: -5311.84231 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.23591 HOMO: -6.85455 LUMO: 0.53062 factor:1 | 1 (-1.02791) | -1 | -1 |
| G: -5311.84231 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.16650 HOMO: -6.49536 LUMO: 0.31021 factor:1 | 1 (-0.95849) | -1 | -1 |
| G: -5311.84231 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.81999 HOMO: -4.97696 LUMO: -0.09252 factor:1 | 1 (-0.61198) | -1 | -1 |
| G: -5311.84231 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.19684 HOMO: -5.31166 LUMO: 0.34286 factor:1 | 1 (-0.98883) | -1 | -1 |
| G: -5311.84231 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.95011 HOMO: -6.42461 LUMO: 0.74287 factor:1 | 1 (-0.74211) | -1 | -1 |
| G: -5311.84231 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.75980 HOMO: -6.59604 LUMO: 0.62858 factor:1 | 1 (-0.55179) | -1 | -1 |
| G: -5311.84231 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.04078 HOMO: -6.45998 LUMO: -0.61770 factor:1 | 1 (-0.83278) | -1 | -1 |
| G: -5311.84231 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.98805 HOMO: -6.75659 LUMO: -0.34014 factor:1 | 1 (-0.78004) | -1 | -1 |
| G: -5311.84231 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11578.40693 HOMO: -6.63958 LUMO: 0.36191 factor:1 | 1 (-2.19892) | -1 | -1 |
| G: -5311.84231 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.71807 HOMO: -5.92936 LUMO: -0.67484 factor:1 | 1 (-1.51007) | -1 | -1 |
| G: -5311.84231 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.81658 HOMO: -5.67630 LUMO: 1.80956 factor:1 | 1 (-1.60857) | -1 | -1 |
| G: -5311.84231 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11578.02926 HOMO: -6.50352 LUMO: -0.78369 factor:1 | 1 (-1.82126) | -1 | -1 |
| G: -5311.84231 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11578.34372 HOMO: -6.35930 LUMO: -0.75648 factor:1 | 1 (-2.13571) | -1 | -1 |
| G: -5311.84231 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11578.21977 HOMO: -6.74298 LUMO: 0.48980 factor:1 | 1 (-2.01176) | -1 | -1 |
| G: -5311.84231 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11578.26497 HOMO: -6.85183 LUMO: 0.15510 factor:1 | 1 (-2.05696) | -1 | -1 |
| G: -5311.84231 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11578.14668 HOMO: -6.90897 LUMO: 0.26123 factor:1 | 1 (-1.93868) | -1 | -1 |
| G: -5311.84231 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.03763 HOMO: -6.85999 LUMO: 0.47892 factor:1 | 1 (-0.82962) | -1 | -1 |
| G: -5311.84231 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.87120 HOMO: -6.69944 LUMO: 0.57416 factor:1 | 1 (-0.66320) | -1 | -1 |
| G: -5311.84231 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.07972 HOMO: -6.74026 LUMO: 0.69933 factor:1 | 1 (-0.87172) | -1 | -1 |
| G: -5311.84231 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11578.43659 HOMO: -6.52801 LUMO: 0.75376 factor:1 | 1 (-2.22859) | -1 | -1 |
| G: -5311.84231 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.90921 HOMO: -7.05863 LUMO: 0.44627 factor:1 | 1 (-1.70120) | -1 | -1 |
| G: -5311.84231 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.80221 HOMO: -6.96339 LUMO: 0.48164 factor:1 | 1 (-1.59421) | -1 | -1 |
| G: -5311.84231 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.90619 HOMO: -6.95795 LUMO: 0.44355 factor:1 | 1 (-1.69818) | -1 | -1 |
| G: -5311.84231 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11578.00703 HOMO: -6.36746 LUMO: 0.58777 factor:1 | 1 (-1.79903) | -1 | -1 |
| G: -5311.84231 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.87946 HOMO: -6.69400 LUMO: 0.40545 factor:1 | 1 (-1.67146) | -1 | -1 |
| G: -5311.84231 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.13657 HOMO: -6.30760 LUMO: -0.66668 factor:1 | 1 (-0.92856) | -1 | -1 |
| G: -5311.84231 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.05120 HOMO: -6.53617 LUMO: -0.64491 factor:1 | 1 (-0.84320) | -1 | -1 |
| G: -5311.84231 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.94410 HOMO: -6.80829 LUMO: 0.17415 factor:1 | 1 (-0.73610) | -1 | -1 |
| G: -5311.84231 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.12138 HOMO: -6.80285 LUMO: 0.73471 factor:1 | 1 (-0.91338) | -1 | -1 |
| G: -5311.84231 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.04282 HOMO: -6.43821 LUMO: 0.21769 factor:1 | 1 (-0.83482) | -1 | -1 |
| G: -5311.84231 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.03874 HOMO: -6.98788 LUMO: 0.10885 factor:1 | 1 (-0.83074) | -1 | -1 |
| G: -5311.84231 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.05523 HOMO: -7.15115 LUMO: 0.40817 factor:1 | 1 (-0.84723) | 1 | 1 |
| G: -5311.84231 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.92949 HOMO: -6.00011 LUMO: -0.98505 factor:1 | 1 (-0.72148) | -1 | -1 |
| G: -5311.84231 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.12590 HOMO: -6.16882 LUMO: -0.77825 factor:1 | 1 (-0.91789) | -1 | -1 |
| G: -5311.84231 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.08603 HOMO: -6.30760 LUMO: 0.34831 factor:1 | 1 (-0.87803) | -1 | -1 |
| G: -5311.84231 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.07700 HOMO: -6.64502 LUMO: 0.63403 factor:1 | 1 (-0.86900) | -1 | -1 |
| G: -5311.84231 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.84032 HOMO: -6.93618 LUMO: 0.96600 factor:1 | 1 (-0.63231) | -1 | -1 |
| G: -5311.84231 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.02666 HOMO: -6.45182 LUMO: 0.16327 factor:1 | 1 (-0.81865) | -1 | -1 |
| G: -5311.84231 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.85101 HOMO: -6.99605 LUMO: 0.20953 factor:1 | 1 (-0.64301) | -1 | -1 |
| G: -5311.84231 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.06329 HOMO: -6.72665 LUMO: 0.32654 factor:1 | 1 (-0.85528) | -1 | -1 |
| G: -5311.84231 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11579.05184 HOMO: -6.38379 LUMO: 0.45443 factor:1 | 1 (-2.84383) | -1 | -1 |
| G: -5311.84231 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11578.24889 HOMO: -6.65318 LUMO: 0.04354 factor:1 | 1 (-2.04088) | -1 | -1 |
| G: -5311.84231 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11578.30391 HOMO: -6.94707 LUMO: -1.68438 factor:1 | 1 (-2.09590) | -1 | -1 |
| G: -5311.84231 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.91966 HOMO: -6.71849 LUMO: 0.15783 factor:1 | 1 (-0.71166) | -1 | -1 |
| G: -5311.84231 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.90990 HOMO: -6.97156 LUMO: 0.43266 factor:1 | 1 (-0.70189) | -1 | -1 |
| G: -5311.84231 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.92821 HOMO: -6.91441 LUMO: -0.54695 factor:1 | 1 (-0.72020) | -1 | -1 |
| G: -5311.84231 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.01300 HOMO: -6.74842 LUMO: -0.76192 factor:1 | 1 (-0.80499) | -1 | -1 |
| G: -5311.84231 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11578.36530 HOMO: -6.70489 LUMO: 0.19048 factor:1 | 1 (-2.15729) | -1 | -1 |
| G: -5311.84231 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.72863 HOMO: -7.25728 LUMO: 0.33470 factor:1 | 1 (-1.52063) | 1 | -1 |
| G: -5311.84231 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.93634 HOMO: -6.96339 LUMO: 0.55511 factor:1 | 1 (-1.72833) | -1 | -1 |
| G: -5311.84231 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.90281 HOMO: -6.77564 LUMO: 0.72382 factor:1 | 1 (-1.69481) | -1 | -1 |
| G: -5311.84231 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.89751 HOMO: -6.75387 LUMO: 0.39729 factor:1 | 1 (-1.68950) | -1 | -1 |
| G: -5311.84231 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.93692 HOMO: -7.00149 LUMO: 0.06531 factor:1 | 1 (-0.72891) | -1 | -1 |
| G: -5311.84231 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.06900 HOMO: -7.09945 LUMO: 0.33470 factor:1 | 1 (-0.86100) | 1 | 1 |
| G: -5311.84231 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.92396 HOMO: -7.20830 LUMO: 0.59593 factor:1 | 1 (-0.71596) | 1 | 1 |
| G: -5311.84231 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.15140 HOMO: -6.40556 LUMO: 0.56600 factor:1 | 1 (-0.94339) | -1 | -1 |
| G: -5311.84231 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.18797 HOMO: -6.77291 LUMO: 0.73471 factor:1 | 1 (-0.97996) | -1 | -1 |
| G: -5311.84231 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.46615 HOMO: -6.65046 LUMO: 0.09796 factor:1 | 1 (-1.25815) | -1 | -1 |
| G: -5311.84231 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.13589 HOMO: -6.95795 LUMO: 0.22313 factor:1 | 1 (-0.92788) | -1 | -1 |
| G: -5311.84231 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.33159 HOMO: -6.85727 LUMO: 0.04626 factor:1 | 1 (-1.12359) | -1 | -1 |
| G: -5311.84231 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.22342 HOMO: -7.27360 LUMO: 0.42178 factor:1 | 1 (-1.01542) | 1 | 1 |
| G: -5311.84231 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.13433 HOMO: -6.78924 LUMO: -0.13334 factor:1 | 1 (-0.92633) | -1 | -1 |
| G: -5311.84231 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.29834 HOMO: -6.63141 LUMO: 0.38368 factor:1 | 1 (-1.09033) | -1 | -1 |
| G: -5311.84231 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.22571 HOMO: -6.92258 LUMO: 0.39184 factor:1 | 1 (-1.01771) | -1 | -1 |
| G: -5311.84231 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.12233 HOMO: -6.19331 LUMO: -0.46804 factor:1 | 1 (-0.91433) | -1 | -1 |
| G: -5311.84231 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.17338 HOMO: -7.26544 LUMO: -0.05442 factor:1 | 1 (-0.96538) | 1 | 1 |
| G: -5311.84231 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.99752 HOMO: -7.09401 LUMO: 0.30749 factor:1 | 1 (-0.78951) | 1 | 1 |
| G: -5311.84231 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.02682 HOMO: -6.14705 LUMO: -0.88709 factor:1 | 1 (-0.81882) | -1 | -1 |
| G: -5311.84231 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.08987 HOMO: -6.53617 LUMO: -0.28572 factor:1 | 1 (-0.88187) | -1 | -1 |
| G: -5311.84231 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.17028 HOMO: -6.37291 LUMO: -0.67212 factor:1 | 1 (-0.96228) | -1 | -1 |
| G: -5311.84231 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.28193 HOMO: -6.65591 LUMO: 0.03810 factor:1 | 1 (-1.07392) | -1 | -1 |
| G: -5311.84231 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.68126 HOMO: -7.11034 LUMO: 0.75103 factor:1 | 1 (-1.47325) | 1 | 1 |
| G: -5311.84231 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.87073 HOMO: -6.85183 LUMO: -0.05987 factor:1 | 1 (-1.66272) | -1 | -1 |
| G: -5311.84231 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.64139 HOMO: -6.70761 LUMO: -0.05442 factor:1 | 1 (-1.43339) | -1 | -1 |
| G: -5311.84231 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.89272 HOMO: -6.23413 LUMO: 0.06259 factor:1 | 1 (-1.68471) | -1 | -1 |
| G: -5311.84231 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.62999 HOMO: -6.55794 LUMO: 0.74015 factor:1 | 1 (-1.42199) | -1 | -1 |
| G: -5311.84231 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.95459 HOMO: -7.27905 LUMO: 0.26939 factor:1 | 1 (-1.74659) | 1 | 1 |
| G: -5311.84231 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.05490 HOMO: -6.34842 LUMO: -0.86804 factor:1 | 1 (-0.84690) | -1 | -1 |
| G: -5311.84231 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.99806 HOMO: -6.27222 LUMO: 1.46125 factor:1 | 1 (-0.79006) | -1 | -1 |
| G: -5311.84231 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.06497 HOMO: -6.65046 LUMO: 2.04902 factor:1 | 1 (-0.85697) | -1 | -1 |
| G: -5311.84231 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.12217 HOMO: -7.11850 LUMO: -1.14016 factor:1 | 1 (-0.91417) | 1 | -1 |
| G: -5311.84231 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.08105 HOMO: -6.88720 LUMO: -1.20274 factor:1 | 1 (-0.87305) | -1 | -1 |
| G: -5311.84231 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.15738 HOMO: -6.69400 LUMO: -0.31565 factor:1 | 1 (-0.94938) | -1 | -1 |
| G: -5311.84231 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.20478 HOMO: -6.95523 LUMO: -1.55377 factor:1 | 1 (-0.99678) | -1 | -1 |
| G: -5311.84231 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.15923 HOMO: -6.41372 LUMO: -0.83539 factor:1 | 1 (-0.95123) | -1 | -1 |
| G: -5311.84231 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.50906 HOMO: -6.13889 LUMO: -0.90070 factor:1 | 1 (-1.30106) | -1 | -1 |
| G: -5311.84231 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.31507 HOMO: -6.44366 LUMO: -0.55511 factor:1 | 1 (-1.10707) | -1 | -1 |
| G: -5311.84231 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.22440 HOMO: -6.10079 LUMO: -0.71022 factor:1 | 1 (-1.01640) | -1 | -1 |
| G: -5311.84231 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.26255 HOMO: -6.90353 LUMO: -0.64763 factor:1 | 1 (-1.05455) | -1 | -1 |
| G: -5311.84231 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.25654 HOMO: -6.65046 LUMO: -0.82450 factor:1 | 1 (-1.04854) | -1 | -1 |
| G: -5311.84231 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.12729 HOMO: -6.81645 LUMO: -0.85444 factor:1 | 1 (-0.91928) | -1 | -1 |
| G: -5311.84231 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.22789 HOMO: -6.20692 LUMO: 1.30887 factor:1 | 1 (-1.01988) | -1 | -1 |
| G: -5311.84231 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.18367 HOMO: -5.96201 LUMO: 1.33880 factor:1 | 1 (-0.97566) | -1 | -1 |
| G: -5311.84231 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.06089 HOMO: -6.52529 LUMO: 1.58914 factor:1 | 1 (-0.85289) | -1 | -1 |
| G: -5311.84231 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.70915 HOMO: -6.58516 LUMO: 1.97555 factor:1 | 1 (-1.50114) | -1 | -1 |
| G: -5311.84231 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.97250 HOMO: -6.84366 LUMO: 0.15783 factor:1 | 1 (-1.76450) | -1 | -1 |
| G: -5311.84231 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.98733 HOMO: -6.45726 LUMO: 0.42994 factor:1 | 1 (-1.77933) | -1 | -1 |
| G: -5311.84231 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.89506 HOMO: -6.75387 LUMO: 0.14422 factor:1 | 1 (-1.68705) | -1 | -1 |
| G: -5311.84231 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11578.00728 HOMO: -6.69944 LUMO: 1.79051 factor:1 | 1 (-1.79927) | -1 | -1 |
| G: -5311.84231 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.81571 HOMO: -6.59876 LUMO: 1.90208 factor:1 | 1 (-1.60770) | -1 | -1 |
| G: -5311.84231 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.80836 HOMO: -7.05863 LUMO: 1.20819 factor:1 | 1 (-1.60036) | -1 | -1 |
| G: -5311.84231 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.17161 HOMO: -6.54978 LUMO: 2.01636 factor:1 | 1 (-0.96361) | -1 | -1 |
| G: -5311.84231 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.31047 HOMO: -5.52119 LUMO: 1.95106 factor:1 | 1 (-1.10247) | -1 | -1 |
| G: -5311.84231 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.22168 HOMO: -6.53617 LUMO: 1.60275 factor:1 | 1 (-1.01368) | -1 | -1 |
| G: -5311.84231 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.13526 HOMO: -6.11440 LUMO: 1.89119 factor:1 | 1 (-0.92726) | -1 | -1 |
| G: -5311.84231 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.58749 HOMO: -7.31986 LUMO: 0.48708 factor:1 | 1 (-1.37948) | 1 | 1 |
| G: -5311.84231 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.71002 HOMO: -6.76475 LUMO: -0.75648 factor:1 | 1 (-1.50201) | -1 | -1 |
| G: -5311.84231 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.74716 HOMO: -6.76747 LUMO: -1.06941 factor:1 | 1 (-1.53916) | -1 | -1 |
| G: -5311.84231 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.88082 HOMO: -6.87087 LUMO: 0.72927 factor:1 | 1 (-1.67282) | -1 | -1 |
| G: -5311.84231 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.70433 HOMO: -7.00965 LUMO: 0.02177 factor:1 | 1 (-1.49633) | -1 | -1 |
| G: -5311.84231 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.57698 HOMO: -6.54706 LUMO: -0.03265 factor:1 | 1 (-1.36898) | -1 | -1 |
| G: -5311.84231 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.69598 HOMO: -6.62325 LUMO: -0.63675 factor:1 | 1 (-1.48797) | -1 | -1 |
| G: -5311.84231 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.75065 HOMO: -7.03414 LUMO: -1.24084 factor:1 | 1 (-1.54264) | -1 | -1 |
| G: -5311.84231 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.51976 HOMO: -7.04503 LUMO: -0.10068 factor:1 | 1 (-1.31175) | -1 | -1 |
| G: -5311.84231 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.58476 HOMO: -6.67223 LUMO: 0.03537 factor:1 | 1 (-1.37676) | -1 | -1 |
| G: -5311.84231 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.88763 HOMO: -6.82734 LUMO: 0.58777 factor:1 | 1 (-1.67962) | -1 | -1 |
| G: -5311.84231 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.91780 HOMO: -6.84366 LUMO: 0.46531 factor:1 | 1 (-1.70980) | -1 | -1 |
| G: -5311.84231 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.67233 HOMO: -7.03959 LUMO: -1.15104 factor:1 | 1 (-1.46433) | -1 | -1 |
| G: -5311.84231 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.71426 HOMO: -6.91169 LUMO: -0.41361 factor:1 | 1 (-1.50626) | -1 | -1 |
| G: -5311.84231 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11578.38712 HOMO: -7.10217 LUMO: -0.44627 factor:1 | 1 (-2.17912) | 1 | 1 |
| G: -5311.84231 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11579.11660 HOMO: -6.88176 LUMO: -0.19592 factor:1 | 1 (-2.90860) | -1 | -1 |
| G: -5311.84231 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11578.42862 HOMO: -7.21374 LUMO: -0.46531 factor:1 | 1 (-2.22061) | 1 | 1 |
| G: -5311.84231 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.91500 HOMO: -6.54978 LUMO: 0.16871 factor:1 | 1 (-1.70700) | -1 | -1 |
| G: -5311.84231 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.91029 HOMO: -6.71305 LUMO: -0.13061 factor:1 | 1 (-1.70229) | -1 | -1 |
| G: -5311.84231 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11578.02831 HOMO: -6.74842 LUMO: -0.36191 factor:1 | 1 (-1.82031) | -1 | -1 |
| G: -5311.84231 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11578.37950 HOMO: -6.74570 LUMO: -0.09796 factor:1 | 1 (-2.17150) | -1 | -1 |
| G: -5311.84231 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11578.22298 HOMO: -6.93890 LUMO: -0.27211 factor:1 | 1 (-2.01498) | -1 | -1 |
| G: -5311.84231 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11578.33262 HOMO: -6.88720 LUMO: -0.18776 factor:1 | 1 (-2.12461) | -1 | -1 |
| G: -5311.84231 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.01199 HOMO: -6.74842 LUMO: 0.02993 factor:1 | 1 (-0.80399) | -1 | -1 |
| G: -5311.84231 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.90432 HOMO: -6.70216 LUMO: 0.01361 factor:1 | 1 (-0.69631) | -1 | -1 |
| G: -5311.84231 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.92502 HOMO: -6.90625 LUMO: 0.00544 factor:1 | 1 (-0.71702) | -1 | -1 |
| G: -5311.84231 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.15861 HOMO: -6.18243 LUMO: 0.25851 factor:1 | 1 (-0.95060) | -1 | -1 |
| G: -5311.84231 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11578.59148 HOMO: -6.32937 LUMO: -0.20953 factor:1 | 1 (-2.38347) | -1 | -1 |
| G: -5311.84231 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.94219 HOMO: -6.78108 LUMO: 0.00544 factor:1 | 1 (-1.73418) | -1 | -1 |
| G: -5311.84231 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.91201 HOMO: -5.97562 LUMO: 0.28572 factor:1 | 1 (-1.70400) | -1 | -1 |
| G: -5311.84231 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.96205 HOMO: -5.97290 LUMO: -0.18504 factor:1 | 1 (-1.75405) | -1 | -1 |
| G: -5311.84231 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.99577 HOMO: -6.12800 LUMO: 0.42178 factor:1 | 1 (-0.78777) | -1 | -1 |
| G: -5311.84231 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.90045 HOMO: -6.24229 LUMO: -0.00816 factor:1 | 1 (-0.69245) | -1 | -1 |
| G: -5311.84231 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.05071 HOMO: -6.61781 LUMO: 0.12789 factor:1 | 1 (-0.84271) | -1 | -1 |
| G: -5311.84231 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.38057 HOMO: -6.70489 LUMO: 0.14694 factor:1 | 1 (-1.17257) | -1 | -1 |
| G: -5311.84231 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.16176 HOMO: -6.86543 LUMO: -0.21225 factor:1 | 1 (-0.95376) | -1 | -1 |
| G: -5311.84231 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.94481 HOMO: -6.90081 LUMO: -0.20136 factor:1 | 1 (-0.73680) | -1 | -1 |
| G: -5311.84231 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.86679 HOMO: -7.12938 LUMO: -0.25851 factor:1 | 1 (-0.65879) | 1 | 1 |
| G: -5311.84231 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.16906 HOMO: -6.93074 LUMO: -0.26667 factor:1 | 1 (-0.96105) | -1 | -1 |
| G: -5311.84231 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.93460 HOMO: -7.00421 LUMO: -0.31021 factor:1 | 1 (-0.72660) | -1 | -1 |
| G: -5311.84231 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.21706 HOMO: -7.10761 LUMO: -0.17415 factor:1 | 1 (-1.00905) | 1 | 1 |
| G: -5311.84231 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.88181 HOMO: -8.21240 LUMO: 0.05987 factor:1 | 1 (-0.67381) | 1 | 1 |
| G: -5311.84231 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.90274 HOMO: -7.14843 LUMO: -0.46531 factor:1 | 1 (-0.69473) | 1 | -1 |
| G: -5311.84231 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.03129 HOMO: -6.80829 LUMO: -0.29933 factor:1 | 1 (-0.82328) | -1 | -1 |
| G: -5311.84231 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.05471 HOMO: -6.84094 LUMO: -0.53606 factor:1 | 1 (-0.84671) | -1 | -1 |
| G: -5311.84231 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.27061 HOMO: -6.81917 LUMO: -0.26667 factor:1 | 1 (-1.06260) | -1 | -1 |
| G: -5311.84231 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.14631 HOMO: -6.85727 LUMO: -1.20002 factor:1 | 1 (-0.93830) | -1 | -1 |
| G: -5311.84231 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.00557 HOMO: -6.39468 LUMO: -1.06941 factor:1 | 1 (-0.79757) | -1 | -1 |
| G: -5311.84231 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.11578 HOMO: -6.00827 LUMO: -1.94017 factor:1 | 1 (-0.90777) | -1 | -1 |
| G: -5311.84231 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.31690 HOMO: -6.80829 LUMO: 0.18504 factor:1 | 1 (-1.10889) | -1 | -1 |
| G: -5311.84231 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.00252 HOMO: -6.54434 LUMO: -0.95784 factor:1 | 1 (-0.79452) | -1 | -1 |
| G: -5311.84231 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.12522 HOMO: -6.45454 LUMO: -0.07347 factor:1 | 1 (-0.91721) | -1 | -1 |
| G: -5311.84231 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.01020 HOMO: -5.33887 LUMO: 1.11839 factor:1 | 1 (-0.80219) | -1 | -1 |
| G: -5311.84231 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.08067 HOMO: -5.75249 LUMO: 0.70477 factor:1 | 1 (-0.87267) | -1 | -1 |
| G: -5311.84231 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.06127 HOMO: -5.64092 LUMO: 0.87076 factor:1 | 1 (-0.85327) | -1 | -1 |
| G: -5311.84231 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.15706 HOMO: -5.14295 LUMO: 1.06124 factor:1 | 1 (-0.94905) | -1 | -1 |
| G: -5311.84231 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.65244 HOMO: -5.05043 LUMO: 1.21091 factor:1 | 1 (-1.44443) | -1 | -1 |
| G: -5311.84231 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.76240 HOMO: -5.05588 LUMO: 1.02859 factor:1 | 1 (-1.55440) | -1 | -1 |
| G: -5311.84231 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.95296 HOMO: -5.76337 LUMO: 0.79457 factor:1 | 1 (-1.74496) | -1 | -1 |
| G: -5311.84231 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.53309 HOMO: -5.01506 LUMO: 1.00138 factor:1 | 1 (-1.32509) | -1 | -1 |
| G: -5311.84231 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.78809 HOMO: -4.84363 LUMO: 1.53744 factor:1 | 1 (-1.58008) | -1 | -1 |
| G: -5311.84231 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.64134 HOMO: -5.17833 LUMO: 1.45309 factor:1 | 1 (-1.43333) | -1 | -1 |
| G: -5311.84231 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11578.02616 HOMO: -5.13751 LUMO: 0.51157 factor:1 | 1 (-1.81816) | -1 | -1 |
| G: -5311.84231 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.81554 HOMO: -5.56473 LUMO: 0.32109 factor:1 | 1 (-1.60754) | -1 | -1 |
| G: -5311.84231 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.89647 HOMO: -4.69941 LUMO: 1.14016 factor:1 | 1 (-1.68847) | -1 | -1 |
| G: -5311.84231 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.96118 HOMO: -4.49260 LUMO: 1.86398 factor:1 | 1 (-1.75318) | -1 | -1 |
| G: -5311.84231 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.97621 HOMO: -4.32117 LUMO: 1.68438 factor:1 | 1 (-0.76820) | -1 | -1 |
| G: -5311.84231 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.02353 HOMO: -4.44906 LUMO: 1.37690 factor:1 | 1 (-0.81553) | -1 | -1 |
| G: -5311.84231 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.14419 HOMO: -4.62049 LUMO: 1.34968 factor:1 | 1 (-0.93618) | -1 | -1 |
| G: -5311.84231 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.08429 HOMO: -4.59600 LUMO: 1.58370 factor:1 | 1 (-0.87629) | -1 | -1 |
| G: -5311.84231 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.99433 HOMO: -4.98785 LUMO: 1.46669 factor:1 | 1 (-0.78633) | -1 | -1 |
| G: -5311.84231 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.78886 HOMO: -5.06676 LUMO: 1.27349 factor:1 | 1 (-0.58085) | -1 | -1 |
| G: -5311.84231 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.83689 HOMO: -5.09125 LUMO: 1.13471 factor:1 | 1 (-0.62888) | -1 | -1 |
| G: -5311.84231 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.91945 HOMO: -4.84635 LUMO: 1.33608 factor:1 | 1 (-0.71144) | -1 | -1 |
| G: -5311.84231 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.97485 HOMO: -4.94431 LUMO: 1.18370 factor:1 | 1 (-0.76684) | -1 | -1 |
| G: -5311.84231 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.14516 HOMO: -4.92526 LUMO: 1.39867 factor:1 | 1 (-0.93716) | -1 | -1 |
| G: -5311.84231 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.85101 HOMO: -5.71983 LUMO: 0.60137 factor:1 | 1 (-0.64301) | -1 | -1 |
| G: -5311.84231 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.75041 HOMO: -5.10486 LUMO: 1.05580 factor:1 | 1 (-0.54240) | -1 | -1 |
| G: -5311.84231 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.88045 HOMO: -5.20282 LUMO: 1.01226 factor:1 | 1 (-0.67245) | -1 | -1 |
| G: -5311.84231 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.78189 HOMO: -4.98513 LUMO: 1.53744 factor:1 | 1 (-0.57389) | -1 | -1 |
| G: -5311.84231 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.06329 HOMO: -5.67085 LUMO: 0.17687 factor:1 | 1 (-0.85528) | -1 | -1 |
| G: -5311.84231 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.90037 HOMO: -5.87222 LUMO: 0.12517 factor:1 | 1 (-0.69237) | -1 | -1 |
| G: -5311.84231 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.05787 HOMO: -5.20826 LUMO: 0.91702 factor:1 | 1 (-0.84987) | -1 | -1 |
| G: -5311.84231 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11578.95440 HOMO: -5.94569 LUMO: 0.63130 factor:1 | 1 (-2.74639) | -1 | -1 |
| G: -5311.84231 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11578.00401 HOMO: -5.35792 LUMO: 0.91430 factor:1 | 1 (-1.79601) | -1 | -1 |
| G: -5311.84231 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11578.22633 HOMO: -5.36336 LUMO: 1.44220 factor:1 | 1 (-2.01832) | -1 | -1 |
| G: -5311.84231 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11578.35074 HOMO: -5.83412 LUMO: 0.71294 factor:1 | 1 (-2.14273) | -1 | -1 |
| G: -5311.84231 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.72037 HOMO: -4.97696 LUMO: 1.72792 factor:1 | 1 (-0.51236) | -1 | -1 |
| G: -5311.84231 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.85237 HOMO: -5.55929 LUMO: 0.23130 factor:1 | 1 (-0.64437) | -1 | -1 |
| G: -5311.84231 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.97158 HOMO: -5.71167 LUMO: 0.47348 factor:1 | 1 (-0.76358) | -1 | -1 |
| G: -5311.84231 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.81248 HOMO: -7.31986 LUMO: -2.54699 factor:1 | 1 (-0.60447) | -1 | -1 |
| G: -5311.84231 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.69759 HOMO: -5.34704 LUMO: 1.19730 factor:1 | 1 (-0.48959) | -1 | -1 |
| G: -5311.84231 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11578.44543 HOMO: -5.45860 LUMO: 0.80818 factor:1 | 1 (-2.23743) | -1 | -1 |
| G: -5311.84231 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.65519 HOMO: -5.12663 LUMO: 1.20274 factor:1 | 1 (-1.44718) | -1 | -1 |
| G: -5311.84231 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.75337 HOMO: -5.37153 LUMO: 1.05580 factor:1 | 1 (-1.54536) | -1 | -1 |
| G: -5311.84231 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.83933 HOMO: -5.47221 LUMO: 0.97961 factor:1 | 1 (-1.63132) | -1 | -1 |
| G: -5311.84231 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.96779 HOMO: -5.06948 LUMO: 1.12111 factor:1 | 1 (-1.75979) | -1 | -1 |
| G: -5311.84231 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.95855 HOMO: -5.19737 LUMO: 1.25444 factor:1 | 1 (-0.75054) | -1 | -1 |
| G: -5311.84231 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.21649 HOMO: -5.27901 LUMO: 1.00682 factor:1 | 1 (-1.00848) | -1 | -1 |
| G: -5311.84231 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.91822 HOMO: -5.38513 LUMO: 0.49253 factor:1 | 1 (-0.71022) | -1 | -1 |
| G: -5311.84231 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.98994 HOMO: -5.12390 LUMO: 1.22995 factor:1 | 1 (-1.78194) | -1 | -1 |
| G: -5311.84231 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.99277 HOMO: -5.31438 LUMO: 0.70205 factor:1 | 1 (-1.78477) | -1 | -1 |
| G: -5311.84231 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.87527 HOMO: -5.17561 LUMO: 1.04492 factor:1 | 1 (-1.66727) | -1 | -1 |
| G: -5311.84231 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.86178 HOMO: -4.94431 LUMO: 1.52656 factor:1 | 1 (-1.65377) | -1 | -1 |
| G: -5311.84231 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.93106 HOMO: -5.13751 LUMO: 0.93879 factor:1 | 1 (-1.72305) | -1 | -1 |
| G: -5311.84231 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11578.52731 HOMO: -5.49942 LUMO: 0.97689 factor:1 | 1 (-2.31931) | -1 | -1 |
| G: -5311.84231 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.20008 HOMO: -5.79058 LUMO: 0.53879 factor:1 | 1 (-0.99207) | -1 | -1 |
| G: -5311.84231 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11578.21245 HOMO: -5.36881 LUMO: 1.56465 factor:1 | 1 (-2.00445) | -1 | -1 |
| G: -5311.84231 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11578.08701 HOMO: -4.67492 LUMO: 1.32792 factor:1 | 1 (-1.87900) | -1 | -1 |
| G: -5311.84231 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.99424 HOMO: -4.60145 LUMO: 1.19458 factor:1 | 1 (-1.78624) | -1 | -1 |
| G: -5311.84231 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.67342 HOMO: -4.49260 LUMO: 1.60547 factor:1 | 1 (-1.46541) | -1 | -1 |
| G: -5311.84231 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.91821 HOMO: -4.65043 LUMO: 1.34696 factor:1 | 1 (-1.71021) | -1 | -1 |
| G: -5311.84231 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11578.06709 HOMO: -4.77560 LUMO: 1.35241 factor:1 | 1 (-1.85908) | -1 | -1 |
| G: -5311.84231 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.82091 HOMO: -4.94431 LUMO: 1.17825 factor:1 | 1 (-1.61290) | -1 | -1 |
| G: -5311.84231 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.66515 HOMO: -4.87084 LUMO: 1.41771 factor:1 | 1 (-1.45714) | -1 | -1 |
| G: -5311.84231 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.37486 HOMO: -5.34432 LUMO: 1.16737 factor:1 | 1 (-1.16685) | -1 | -1 |
| G: -5311.84231 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.47339 HOMO: -4.94975 LUMO: 1.67622 factor:1 | 1 (-1.26538) | -1 | -1 |
| G: -5311.84231 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.45910 HOMO: -4.81369 LUMO: 1.14288 factor:1 | 1 (-1.25110) | -1 | -1 |
| G: -5311.84231 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.26756 HOMO: -5.22459 LUMO: 0.29660 factor:1 | 1 (-1.05956) | -1 | -1 |
| G: -5311.84231 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.88371 HOMO: -5.21642 LUMO: 0.37824 factor:1 | 1 (-1.67570) | -1 | -1 |
| G: -5311.84231 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.62332 HOMO: -5.00417 LUMO: 1.01226 factor:1 | 1 (-1.41532) | -1 | -1 |
| G: -5311.84231 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.62354 HOMO: -5.46677 LUMO: 0.10612 factor:1 | 1 (-1.41554) | -1 | -1 |
| G: -5311.84231 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.48607 HOMO: -5.51303 LUMO: 0.54151 factor:1 | 1 (-1.27806) | -1 | -1 |
| G: -5311.84231 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.54626 HOMO: -5.63004 LUMO: 0.17960 factor:1 | 1 (-1.33826) | -1 | -1 |
| G: -5311.84231 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.46640 HOMO: -4.79193 LUMO: 1.12111 factor:1 | 1 (-1.25839) | -1 | -1 |
| G: -5311.84231 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.40193 HOMO: -5.43411 LUMO: 0.45987 factor:1 | 1 (-1.19393) | -1 | -1 |
| G: -5311.84231 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.17673 HOMO: -7.06135 LUMO: -2.13881 factor:1 | 1 (-0.96873) | 1 | 1 |
| G: -5311.84231 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.32386 HOMO: -5.33071 LUMO: 1.14016 factor:1 | 1 (-1.11586) | -1 | -1 |
| G: -5311.84231 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.29080 HOMO: -7.12394 LUMO: -0.03810 factor:1 | 1 (-1.08280) | 1 | 1 |
| G: -5311.84231 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.73803 HOMO: -7.20558 LUMO: -2.50889 factor:1 | 1 (-0.53002) | 1 | 1 |
| G: -5311.84231 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.10696 HOMO: -7.26816 LUMO: -2.11432 factor:1 | 1 (-0.89896) | 1 | 1 |
| G: -5311.84231 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.27080 HOMO: -7.89674 LUMO: 0.31021 factor:1 | 1 (-1.06280) | 1 | 1 |
| G: -5311.84231 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.31456 HOMO: -7.26544 LUMO: 0.22858 factor:1 | 1 (-1.10655) | 1 | 1 |
| G: -5311.84231 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.44906 HOMO: -7.12666 LUMO: -0.02449 factor:1 | 1 (-1.24106) | 1 | 1 |
| G: -5311.84231 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.46435 HOMO: -7.68722 LUMO: 0.71838 factor:1 | 1 (-1.25635) | 1 | 1 |
| G: -5311.84231 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.85116 HOMO: -6.86271 LUMO: -0.96056 factor:1 | 1 (-1.64316) | -1 | -1 |
| G: -5311.84231 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11578.06088 HOMO: -7.07496 LUMO: -1.11839 factor:1 | 1 (-1.85288) | 1 | 1 |
| G: -5311.84231 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11578.02202 HOMO: -7.06952 LUMO: -2.08439 factor:1 | 1 (-1.81402) | 1 | 1 |
| G: -5311.84231 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11578.21381 HOMO: -6.60965 LUMO: -2.11977 factor:1 | 1 (-2.00581) | -1 | -1 |
| G: -5311.84231 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.77380 HOMO: -6.87360 LUMO: -1.85854 factor:1 | 1 (-1.56580) | -1 | -1 |
| G: -5311.84231 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11578.00850 HOMO: -7.67089 LUMO: -0.24762 factor:1 | 1 (-1.80050) | 1 | 1 |
| G: -5311.84231 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.95089 HOMO: -6.45726 LUMO: -1.86398 factor:1 | 1 (-1.74289) | -1 | -1 |
| G: -5311.84231 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11578.06075 HOMO: -6.91713 LUMO: 0.33198 factor:1 | 1 (-1.85274) | -1 | -1 |
| G: -5311.84231 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.89399 HOMO: -6.83278 LUMO: 0.26667 factor:1 | 1 (-1.68599) | -1 | -1 |
| G: -5311.84231 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11578.14146 HOMO: -6.89264 LUMO: -1.00682 factor:1 | 1 (-1.93345) | -1 | -1 |
| G: -5311.84231 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.70452 HOMO: -6.57427 LUMO: 0.22041 factor:1 | 1 (-1.49652) | -1 | -1 |
| G: -5311.84231 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.86997 HOMO: -7.52123 LUMO: -0.01905 factor:1 | 1 (-1.66196) | 1 | 1 |
| G: -5311.84231 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.77571 HOMO: -7.37429 LUMO: -0.08980 factor:1 | 1 (-1.56770) | 1 | 1 |
| G: -5311.84231 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.81361 HOMO: -7.28449 LUMO: -0.26395 factor:1 | 1 (-1.60561) | 1 | 1 |
| G: -5311.84231 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.86338 HOMO: -6.79740 LUMO: -0.60954 factor:1 | 1 (-1.65538) | -1 | -1 |
| G: -5311.84231 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11578.22701 HOMO: -7.12666 LUMO: -0.60681 factor:1 | 1 (-2.01900) | 1 | 1 |
| G: -5311.84231 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11578.04143 HOMO: -6.96611 LUMO: -0.30477 factor:1 | 1 (-1.83342) | -1 | -1 |
| G: -5311.84231 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11578.00494 HOMO: -7.08040 LUMO: -0.31293 factor:1 | 1 (-1.79693) | 1 | 1 |
| G: -5311.84231 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.23273 HOMO: -6.78924 LUMO: -0.73743 factor:1 | 1 (-1.02473) | -1 | -1 |
| G: -5311.84231 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.31940 HOMO: -7.57293 LUMO: -1.11295 factor:1 | 1 (-1.11139) | 1 | 1 |
| G: -5311.84231 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.90151 HOMO: -7.15932 LUMO: -0.23130 factor:1 | 1 (-0.69351) | 1 | 1 |
| G: -5311.84231 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.00786 HOMO: -7.48585 LUMO: -0.10068 factor:1 | 1 (-0.79985) | 1 | 1 |
| G: -5311.84231 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.24511 HOMO: -7.17020 LUMO: -0.26123 factor:1 | 1 (-1.03711) | 1 | 1 |
| G: -5311.84231 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.43682 HOMO: -7.43143 LUMO: -0.16055 factor:1 | 1 (-1.22881) | 1 | 1 |
| G: -5311.84231 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.83966 HOMO: -7.14843 LUMO: -0.10612 factor:1 | 1 (-0.63166) | 1 | 1 |
| G: -5311.84231 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.07820 HOMO: -6.95523 LUMO: -0.22585 factor:1 | 1 (-0.87019) | -1 | -1 |
| G: -5311.84231 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.27589 HOMO: -7.06680 LUMO: -0.51974 factor:1 | 1 (-1.06788) | 1 | 1 |
| G: -5311.84231 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.84099 HOMO: -6.80829 LUMO: -0.64763 factor:1 | 1 (-1.63298) | -1 | -1 |
| G: -5311.84231 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.84602 HOMO: -7.13210 LUMO: -0.48164 factor:1 | 1 (-1.63802) | 1 | 1 |
| G: -5311.84231 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.77715 HOMO: -7.16204 LUMO: -0.45715 factor:1 | 1 (-1.56914) | 1 | 1 |
| G: -5311.84231 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.77601 HOMO: -7.15115 LUMO: -0.43266 factor:1 | 1 (-1.56800) | 1 | 1 |
| G: -5311.84231 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.84099 HOMO: -7.15932 LUMO: -2.52794 factor:1 | 1 (-1.63298) | -1 | -1 |
| G: -5311.84231 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.76071 HOMO: -7.21102 LUMO: -2.65311 factor:1 | 1 (-1.55271) | -1 | -1 |
| G: -5311.84231 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.82929 HOMO: -6.57427 LUMO: -2.78645 factor:1 | 1 (-1.62128) | -1 | -1 |
| G: -5311.84231 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.83998 HOMO: -6.40828 LUMO: -3.23815 factor:1 | 1 (-1.63198) | -1 | -1 |
| G: -5311.84231 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11578.06382 HOMO: -7.71987 LUMO: -0.20953 factor:1 | 1 (-1.85582) | 1 | 1 |
| G: -5311.84231 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11578.05656 HOMO: -7.47769 LUMO: -0.43810 factor:1 | 1 (-1.84855) | 1 | 1 |
| G: -5311.84231 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.78877 HOMO: -6.68040 LUMO: -2.22589 factor:1 | 1 (-1.58076) | -1 | -1 |
| G: -5311.84231 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.94172 HOMO: -6.92802 LUMO: -1.99187 factor:1 | 1 (-1.73372) | -1 | -1 |
| G: -5311.84231 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.96847 HOMO: -7.73620 LUMO: 0.01633 factor:1 | 1 (-1.76047) | 1 | 1 |
| G: -5311.84231 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.95070 HOMO: -7.28721 LUMO: -0.18504 factor:1 | 1 (-1.74270) | 1 | 1 |
| G: -5311.84231 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.86142 HOMO: -7.49674 LUMO: -0.19864 factor:1 | 1 (-1.65342) | 1 | 1 |
| G: -5311.84231 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.97636 HOMO: -7.10489 LUMO: -2.56331 factor:1 | 1 (-1.76836) | -1 | -1 |
| G: -5311.84231 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.71573 HOMO: -7.36612 LUMO: 0.16055 factor:1 | 1 (-1.50773) | 1 | 1 |
| G: -5311.84231 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11578.05544 HOMO: -7.67633 LUMO: 0.33198 factor:1 | 1 (-1.84744) | 1 | 1 |
| G: -5311.84231 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11578.06317 HOMO: -7.07768 LUMO: -0.27483 factor:1 | 1 (-1.85516) | 1 | 1 |
| G: -5311.84231 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11578.09218 HOMO: -7.32531 LUMO: 0.05442 factor:1 | 1 (-1.88417) | 1 | 1 |
| G: -5311.84231 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.77130 HOMO: -6.79740 LUMO: -1.21635 factor:1 | 1 (-1.56329) | -1 | -1 |
| G: -5311.84231 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.76115 HOMO: -7.14027 LUMO: 0.12517 factor:1 | 1 (-1.55314) | 1 | -1 |
| G: -5311.84231 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11578.03054 HOMO: -7.17292 LUMO: 0.16871 factor:1 | 1 (-1.82254) | 1 | -1 |
| G: -5311.84231 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.76855 HOMO: -7.08312 LUMO: -1.38778 factor:1 | 1 (-1.56055) | 1 | 1 |
| G: -5311.84231 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.89979 HOMO: -6.75387 LUMO: -1.88031 factor:1 | 1 (-1.69179) | -1 | -1 |
| G: -5311.84231 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.75244 HOMO: -7.07768 LUMO: -1.25717 factor:1 | 1 (-1.54444) | 1 | 1 |
| G: -5311.84231 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.68357 HOMO: -6.46543 LUMO: -1.14016 factor:1 | 1 (-1.47556) | -1 | -1 |
| G: -5311.84231 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.96059 HOMO: -7.37973 LUMO: -0.45987 factor:1 | 1 (-0.75259) | 1 | 1 |
| G: -5311.84231 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.28223 HOMO: -7.46408 LUMO: 0.03265 factor:1 | 1 (-1.07422) | 1 | 1 |
| G: -5311.84231 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.07545 HOMO: -7.96477 LUMO: -0.19864 factor:1 | 1 (-0.86744) | 1 | 1 |
| G: -5311.84231 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.03052 HOMO: -6.93890 LUMO: -1.11839 factor:1 | 1 (-0.82252) | -1 | -1 |
| G: -5311.84231 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.86180 HOMO: -7.06408 LUMO: -1.08846 factor:1 | 1 (-1.65380) | 1 | 1 |
| G: -5311.84231 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.72137 HOMO: -7.14027 LUMO: -0.33470 factor:1 | 1 (-1.51336) | 1 | 1 |
| G: -5311.84231 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11578.10442 HOMO: -7.38245 LUMO: 0.10885 factor:1 | 1 (-1.89642) | 1 | 1 |
| G: -5311.84231 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.94834 HOMO: -7.59470 LUMO: -1.21363 factor:1 | 1 (-1.74033) | 1 | 1 |
| G: -5311.84231 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.93908 HOMO: -7.23279 LUMO: -1.23812 factor:1 | 1 (-1.73108) | 1 | 1 |
| G: -5311.84231 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11578.05239 HOMO: -6.90897 LUMO: 0.23402 factor:1 | 1 (-1.84439) | -1 | -1 |
| G: -5311.84231 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.78537 HOMO: -7.36340 LUMO: -0.17143 factor:1 | 1 (-1.57736) | 1 | 1 |
| G: -5311.84231 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.85157 HOMO: -6.61781 LUMO: -0.01361 factor:1 | 1 (-1.64357) | -1 | -1 |
| G: -5311.84231 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11578.03854 HOMO: -6.80013 LUMO: 0.38368 factor:1 | 1 (-1.83054) | -1 | -1 |
| G: -5311.84231 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11578.06763 HOMO: -6.72121 LUMO: -0.95512 factor:1 | 1 (-1.85963) | -1 | -1 |
| G: -5311.84231 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11578.09294 HOMO: -6.24773 LUMO: -0.69933 factor:1 | 1 (-1.88493) | -1 | -1 |
| G: -5311.84231 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.93631 HOMO: -6.56883 LUMO: 0.14694 factor:1 | 1 (-1.72830) | -1 | -1 |
| G: -5311.84231 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.77212 HOMO: -6.51441 LUMO: -1.27621 factor:1 | 1 (-1.56411) | -1 | -1 |
| G: -5311.84231 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.61630 HOMO: -6.91986 LUMO: -1.16737 factor:1 | 1 (-1.40830) | -1 | -1 |
| G: -5311.84231 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.80455 HOMO: -6.17971 LUMO: -0.65307 factor:1 | 1 (-1.59655) | -1 | -1 |
| G: -5311.84231 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.87865 HOMO: -7.22462 LUMO: 0.04354 factor:1 | 1 (-1.67064) | 1 | 1 |
| G: -5311.84231 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.74014 HOMO: -7.16204 LUMO: -0.23674 factor:1 | 1 (-1.53214) | 1 | 1 |
| G: -5311.84231 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.56972 HOMO: -6.81645 LUMO: -0.19320 factor:1 | 1 (-1.36171) | -1 | -1 |
| G: -5311.84231 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.44552 HOMO: -6.69400 LUMO: 0.04082 factor:1 | 1 (-1.23752) | -1 | -1 |
| G: -5311.84231 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.59935 HOMO: -6.63141 LUMO: -0.22858 factor:1 | 1 (-1.39135) | -1 | -1 |
| G: -5311.84231 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.52329 HOMO: -6.92258 LUMO: -1.11295 factor:1 | 1 (-1.31529) | -1 | -1 |
| G: -5311.84231 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.71383 HOMO: -6.60148 LUMO: -1.13744 factor:1 | 1 (-1.50582) | -1 | -1 |
| G: -5311.84231 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.42596 HOMO: -6.78108 LUMO: -0.82450 factor:1 | 1 (-1.21795) | -1 | -1 |
| G: -5311.84231 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.65685 HOMO: -7.05591 LUMO: -0.97145 factor:1 | 1 (-1.44884) | -1 | -1 |
| G: -5311.84231 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.50610 HOMO: -6.65318 LUMO: -1.26261 factor:1 | 1 (-1.29809) | -1 | -1 |
| G: -5311.84231 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.60893 HOMO: -6.98244 LUMO: -0.98233 factor:1 | 1 (-1.40092) | -1 | -1 |
| G: -5311.84231 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.82452 HOMO: -7.11850 LUMO: -0.99594 factor:1 | 1 (-1.61652) | 1 | 1 |
| G: -5311.84231 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.53584 HOMO: -6.64230 LUMO: -0.93879 factor:1 | 1 (-1.32783) | -1 | -1 |
| G: -5311.84231 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.48803 HOMO: -6.62053 LUMO: -1.22451 factor:1 | 1 (-1.28002) | -1 | -1 |
| G: -5311.84231 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.43894 HOMO: -7.02598 LUMO: -0.85172 factor:1 | 1 (-1.23093) | -1 | -1 |
| G: -5311.84231 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.72343 HOMO: -7.06680 LUMO: -0.89253 factor:1 | 1 (-1.51543) | 1 | 1 |
| G: -5311.84231 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.63081 HOMO: -7.17292 LUMO: 0.00272 factor:1 | 1 (-1.42280) | 1 | 1 |
| G: -5311.84231 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.70928 HOMO: -7.03142 LUMO: -0.35103 factor:1 | 1 (-1.50128) | -1 | -1 |
| G: -5311.84231 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.74349 HOMO: -6.96884 LUMO: -0.09796 factor:1 | 1 (-1.53548) | -1 | -1 |
| G: -5311.84231 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.83481 HOMO: -6.56339 LUMO: -0.99322 factor:1 | 1 (-1.62681) | -1 | -1 |
| G: -5311.84231 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11578.05411 HOMO: -7.08857 LUMO: -0.17687 factor:1 | 1 (-1.84610) | 1 | 1 |
| G: -5311.84231 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.79761 HOMO: -7.05863 LUMO: -0.22041 factor:1 | 1 (-1.58961) | -1 | -1 |
| G: -5311.84231 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.76428 HOMO: -7.15115 LUMO: -0.17960 factor:1 | 1 (-1.55627) | 1 | 1 |
| G: -5311.84231 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.75108 HOMO: -6.67495 LUMO: -0.96600 factor:1 | 1 (-1.54308) | -1 | -1 |
| G: -5311.84231 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.91136 HOMO: -6.74026 LUMO: -1.79867 factor:1 | 1 (-1.70335) | -1 | -1 |
| G: -5311.84231 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.70488 HOMO: -6.73482 LUMO: -1.78235 factor:1 | 1 (-1.49687) | -1 | -1 |
| G: -5311.84231 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.78934 HOMO: -6.09807 LUMO: 0.16871 factor:1 | 1 (-1.58134) | -1 | -1 |
| G: -5311.84231 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.48343 HOMO: -6.72393 LUMO: 0.27211 factor:1 | 1 (-1.27542) | -1 | -1 |
| G: -5311.84231 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.43818 HOMO: -6.40556 LUMO: -0.04354 factor:1 | 1 (-1.23017) | -1 | -1 |
| G: -5311.84231 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.54229 HOMO: -6.56883 LUMO: 0.22041 factor:1 | 1 (-1.33428) | -1 | -1 |
| G: -5311.84231 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.43543 HOMO: -7.22462 LUMO: 0.15783 factor:1 | 1 (-1.22742) | 1 | 1 |
| G: -5311.84231 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.34990 HOMO: -6.83550 LUMO: 0.19320 factor:1 | 1 (-1.14190) | -1 | -1 |
| G: -5311.84231 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.39061 HOMO: -7.26816 LUMO: -0.07619 factor:1 | 1 (-1.18261) | 1 | -1 |
| G: -5311.84231 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.64136 HOMO: -7.13483 LUMO: 0.33198 factor:1 | 1 (-1.43336) | 1 | 1 |
| G: -5311.84231 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.42732 HOMO: -6.58243 LUMO: -0.26395 factor:1 | 1 (-1.21931) | -1 | -1 |
| G: -5311.84231 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.73405 HOMO: -7.38517 LUMO: 0.17143 factor:1 | 1 (-1.52604) | 1 | 1 |
| G: -5311.84231 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.48950 HOMO: -6.80013 LUMO: 0.25851 factor:1 | 1 (-1.28149) | -1 | -1 |
| G: -5311.84231 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.33015 HOMO: -6.96611 LUMO: 0.11429 factor:1 | 1 (-1.12214) | -1 | -1 |
| G: -5311.84231 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.27763 HOMO: -6.51713 LUMO: -1.14560 factor:1 | 1 (-1.06963) | -1 | -1 |
| G: -5311.84231 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.17774 HOMO: -7.15387 LUMO: -0.35647 factor:1 | 1 (-0.96973) | 1 | 1 |
| G: -5311.84231 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.93550 HOMO: -5.26540 LUMO: 1.26805 factor:1 | 1 (-0.72750) | -1 | -1 |
| G: -5311.84231 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.42231 HOMO: -6.76475 LUMO: -0.16327 factor:1 | 1 (-1.21431) | -1 | -1 |
| G: -5311.84231 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.22381 HOMO: -6.55250 LUMO: -0.71838 factor:1 | 1 (-1.01580) | -1 | -1 |
| G: -5311.84231 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.11708 HOMO: -6.76203 LUMO: -1.08301 factor:1 | 1 (-0.90908) | -1 | -1 |
| G: -5311.84231 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.60969 HOMO: -7.14027 LUMO: -0.01633 factor:1 | 1 (-1.40169) | 1 | 1 |
| G: -5311.84231 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.16239 HOMO: -6.94979 LUMO: -0.93879 factor:1 | 1 (-0.95438) | -1 | -1 |
| G: -5311.84231 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.27962 HOMO: -6.74842 LUMO: 0.31293 factor:1 | 1 (-1.07161) | -1 | -1 |
| G: -5311.84231 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.36359 HOMO: -6.43821 LUMO: 0.05987 factor:1 | 1 (-1.15559) | -1 | -1 |
| G: -5311.84231 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11578.11743 HOMO: -6.60420 LUMO: 0.22585 factor:1 | 1 (-1.90942) | -1 | -1 |
| G: -5311.84231 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11578.01816 HOMO: -6.43821 LUMO: 0.05987 factor:1 | 1 (-1.81016) | -1 | -1 |
| G: -5311.84231 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11578.34641 HOMO: -6.34570 LUMO: 1.43948 factor:1 | 1 (-2.13841) | -1 | -1 |
| G: -5311.84231 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.81614 HOMO: -6.03004 LUMO: 1.21363 factor:1 | 1 (-1.60814) | -1 | -1 |
| G: -5311.84231 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11578.72579 HOMO: -6.68040 LUMO: -0.92247 factor:1 | 1 (-2.51779) | -1 | -1 |
| G: -5311.84231 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11578.20976 HOMO: -6.92530 LUMO: -0.31293 factor:1 | 1 (-2.00175) | -1 | -1 |
| G: -5311.84231 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11578.40336 HOMO: -6.94979 LUMO: -0.19864 factor:1 | 1 (-2.19536) | -1 | -1 |
| G: -5311.84231 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11578.39887 HOMO: -6.80829 LUMO: -0.30477 factor:1 | 1 (-2.19087) | -1 | -1 |
| G: -5311.84231 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11578.77831 HOMO: -7.22734 LUMO: -1.02859 factor:1 | 1 (-2.57031) | 1 | 1 |
| G: -5311.84231 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11578.21773 HOMO: -6.93890 LUMO: -0.72382 factor:1 | 1 (-2.00972) | -1 | -1 |
| G: -5311.84231 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11578.53074 HOMO: -7.27088 LUMO: -0.78097 factor:1 | 1 (-2.32274) | 1 | 1 |
| G: -5311.84231 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11579.08836 HOMO: -7.29809 LUMO: -0.97145 factor:1 | 1 (-2.88035) | 1 | 1 |
| G: -5311.84231 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11578.82120 HOMO: -7.18925 LUMO: -0.94696 factor:1 | 1 (-2.61319) | 1 | 1 |
| G: -5311.84231 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11578.27542 HOMO: -7.33891 LUMO: -0.96873 factor:1 | 1 (-2.06741) | 1 | 1 |
| G: -5311.84231 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11578.38184 HOMO: -7.36068 LUMO: -0.28028 factor:1 | 1 (-2.17384) | 1 | 1 |
| G: -5311.84231 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11578.16682 HOMO: -7.10761 LUMO: -1.14832 factor:1 | 1 (-1.95881) | 1 | 1 |
| G: -5311.84231 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11579.02120 HOMO: -6.94707 LUMO: -0.65307 factor:1 | 1 (-2.81319) | -1 | -1 |
| G: -5311.84231 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11578.83913 HOMO: -6.91713 LUMO: -1.81228 factor:1 | 1 (-2.63112) | -1 | -1 |
| G: -5311.84231 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11578.03351 HOMO: -6.78652 LUMO: -2.01636 factor:1 | 1 (-1.82550) | -1 | -1 |
| G: -5311.84231 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11578.23299 HOMO: -6.52801 LUMO: -1.17553 factor:1 | 1 (-2.02499) | -1 | -1 |
| G: -5311.84231 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.84477 HOMO: -7.54844 LUMO: -1.18642 factor:1 | 1 (-1.63676) | 1 | -1 |
| G: -5311.84231 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.79947 HOMO: -7.52939 LUMO: -1.23812 factor:1 | 1 (-0.59147) | 1 | -1 |
| G: -5311.84231 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.84769 HOMO: -7.94572 LUMO: -0.81634 factor:1 | 1 (-0.63969) | 1 | 1 |
| G: -5311.84231 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.86249 HOMO: -7.55932 LUMO: -0.86260 factor:1 | 1 (-0.65449) | 1 | 1 |
| G: -5311.84231 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.62652 HOMO: -7.72259 LUMO: -1.39050 factor:1 | 1 (-0.41851) | 1 | -1 |
| G: -5311.84231 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.73604 HOMO: -7.11850 LUMO: -1.01498 factor:1 | 1 (-0.52804) | 1 | -1 |
| G: -5311.84231 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.66398 HOMO: -7.09673 LUMO: -1.00954 factor:1 | 1 (-1.45597) | 1 | -1 |
| G: -5311.84231 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.89965 HOMO: -6.06270 LUMO: 0.16327 factor:1 | 1 (-1.69165) | -1 | -1 |
| G: -5311.84231 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.91835 HOMO: -5.71167 LUMO: 0.70477 factor:1 | 1 (-1.71034) | -1 | -1 |
| G: -5311.84231 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.59715 HOMO: -5.38241 LUMO: 0.86260 factor:1 | 1 (-1.38914) | -1 | -1 |
| G: -5311.84231 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.86385 HOMO: -5.67357 LUMO: 1.27621 factor:1 | 1 (-0.65585) | -1 | -1 |
| G: -5311.84231 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.86021 HOMO: -7.56204 LUMO: -0.68573 factor:1 | 1 (-0.65220) | 1 | 1 |
| G: -5311.84231 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.02035 HOMO: -5.57833 LUMO: 1.13199 factor:1 | 1 (-0.81234) | -1 | -1 |
| G: -5311.84231 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.22378 HOMO: -7.58653 LUMO: -0.66124 factor:1 | 1 (-1.01577) | 1 | 1 |
| G: -5311.84231 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.09305 HOMO: -7.91851 LUMO: -1.10206 factor:1 | 1 (-0.88505) | 1 | -1 |
| G: -5311.84231 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.71770 HOMO: -6.48992 LUMO: -1.00138 factor:1 | 1 (-0.50970) | -1 | -1 |
| G: -5311.84231 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.80674 HOMO: -7.09673 LUMO: -0.45171 factor:1 | 1 (-0.59873) | 1 | 1 |
| G: -5311.84231 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.72845 HOMO: -6.63686 LUMO: 0.09252 factor:1 | 1 (-0.52044) | -1 | -1 |
| G: -5311.84231 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.05586 HOMO: -6.84366 LUMO: -0.14422 factor:1 | 1 (-0.84785) | -1 | -1 |
| G: -5311.84231 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.82402 HOMO: -6.93074 LUMO: 0.04354 factor:1 | 1 (-0.61601) | -1 | -1 |
| G: -5311.84231 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.98347 HOMO: -6.90353 LUMO: -0.19864 factor:1 | 1 (-0.77547) | -1 | -1 |
| G: -5311.84231 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.21616 HOMO: -6.59876 LUMO: -0.10068 factor:1 | 1 (-1.00815) | -1 | -1 |
| G: -5311.84231 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.55585 HOMO: -6.74570 LUMO: -0.44627 factor:1 | 1 (-0.34784) | -1 | -1 |
| G: -5311.84231 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.69454 HOMO: -6.60148 LUMO: -0.61770 factor:1 | 1 (-0.48654) | -1 | -1 |
| G: -5311.84231 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.89047 HOMO: -6.55794 LUMO: -1.06941 factor:1 | 1 (-0.68246) | -1 | -1 |
| G: -5311.84231 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.68799 HOMO: -7.12666 LUMO: -0.11973 factor:1 | 1 (-0.47998) | 1 | 1 |
| G: -5311.84231 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.13257 HOMO: -7.21646 LUMO: -0.50069 factor:1 | 1 (-0.92456) | 1 | 1 |
| G: -5311.84231 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.19061 HOMO: -7.27632 LUMO: -1.00682 factor:1 | 1 (-0.98260) | 1 | -1 |
| G: -5311.84231 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.92418 HOMO: -6.74298 LUMO: 0.04354 factor:1 | 1 (-0.71618) | -1 | -1 |
| G: -5311.84231 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.76323 HOMO: -6.37291 LUMO: 0.14150 factor:1 | 1 (-0.55522) | -1 | -1 |
| G: -5311.84231 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.61057 HOMO: -5.61371 LUMO: 1.28438 factor:1 | 1 (-0.40257) | -1 | -1 |
| G: -5311.84231 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11578.08398 HOMO: -5.52119 LUMO: 0.99866 factor:1 | 1 (-1.87598) | -1 | -1 |
| G: -5311.84231 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11579.01891 HOMO: -6.51985 LUMO: -0.10885 factor:1 | 1 (-2.81091) | -1 | -1 |
| G: -5311.84231 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11578.31131 HOMO: -5.61371 LUMO: 0.77280 factor:1 | 1 (-2.10330) | -1 | -1 |
| G: -5311.84231 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11578.02292 HOMO: -5.58922 LUMO: 0.24490 factor:1 | 1 (-1.81492) | -1 | -1 |
| G: -5311.84231 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.78320 HOMO: -6.32665 LUMO: -0.57144 factor:1 | 1 (-0.57519) | -1 | -1 |
| G: -5311.84231 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.75087 HOMO: -6.29127 LUMO: -0.93607 factor:1 | 1 (-0.54287) | -1 | -1 |
| G: -5311.84231 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.07145 HOMO: -5.49670 LUMO: 0.27211 factor:1 | 1 (-0.86344) | -1 | -1 |
| G: -5311.84231 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.99123 HOMO: -5.68990 LUMO: 0.24218 factor:1 | 1 (-0.78323) | -1 | -1 |
| G: -5311.84231 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.66284 HOMO: -5.68174 LUMO: 0.69933 factor:1 | 1 (-0.45484) | -1 | -1 |
| G: -5311.84231 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.77301 HOMO: -5.28173 LUMO: 1.00954 factor:1 | 1 (-1.56501) | -1 | -1 |
| G: -5311.84231 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11578.40494 HOMO: -5.94025 LUMO: 0.73471 factor:1 | 1 (-2.19694) | -1 | -1 |
| G: -5311.84231 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.74382 HOMO: -5.65725 LUMO: 1.28710 factor:1 | 1 (-1.53581) | -1 | -1 |
| G: -5311.84231 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.99171 HOMO: -5.41507 LUMO: 0.87076 factor:1 | 1 (-1.78371) | -1 | -1 |
| G: -5311.84231 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.68654 HOMO: -5.96474 LUMO: 0.29660 factor:1 | 1 (-1.47853) | -1 | -1 |
| G: -5311.84231 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.69530 HOMO: -7.00421 LUMO: 0.08708 factor:1 | 1 (-1.48729) | -1 | -1 |
| G: -5311.84231 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.91348 HOMO: -5.40418 LUMO: 0.90070 factor:1 | 1 (-1.70547) | -1 | -1 |
| G: -5311.84231 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.92741 HOMO: -7.00421 LUMO: -0.30477 factor:1 | 1 (-1.71941) | -1 | -1 |
| G: -5311.84231 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.50670 HOMO: -5.85861 LUMO: 0.74015 factor:1 | 1 (-1.29869) | -1 | -1 |
| G: -5311.84231 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11578.06241 HOMO: -5.71439 LUMO: 0.26395 factor:1 | 1 (-1.85440) | -1 | -1 |
| G: -5311.84231 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.97402 HOMO: -7.13755 LUMO: -0.78369 factor:1 | 1 (-1.76602) | 1 | -1 |
| G: -5311.84231 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11578.26331 HOMO: -7.31442 LUMO: -0.98233 factor:1 | 1 (-2.05530) | 1 | -1 |
| G: -5311.84231 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.73931 HOMO: -7.25728 LUMO: -1.00410 factor:1 | 1 (-0.53130) | 1 | -1 |
| G: -5311.84231 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.83144 HOMO: -7.48585 LUMO: -0.83811 factor:1 | 1 (-0.62344) | 1 | -1 |
| G: -5311.84231 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.57781 HOMO: -7.24911 LUMO: -0.77280 factor:1 | 1 (-0.36980) | 1 | -1 |
| G: -5311.84231 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.89564 HOMO: -7.55116 LUMO: -1.19730 factor:1 | 1 (-0.68763) | 1 | -1 |
| G: -5311.84231 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.04369 HOMO: -5.76881 LUMO: 0.28028 factor:1 | 1 (-0.83569) | -1 | -1 |
| G: -5311.84231 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.61098 HOMO: -5.77153 LUMO: -0.26939 factor:1 | 1 (-0.40297) | -1 | -1 |
| G: -5311.84231 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11578.45460 HOMO: -5.82868 LUMO: 0.36735 factor:1 | 1 (-2.24660) | -1 | -1 |
| G: -5311.84231 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.63078 HOMO: -5.83140 LUMO: -0.17960 factor:1 | 1 (-1.42277) | -1 | -1 |
| G: -5311.84231 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.76730 HOMO: -6.28855 LUMO: 0.01088 factor:1 | 1 (-1.55929) | -1 | -1 |
| G: -5311.84231 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.91810 HOMO: -6.31576 LUMO: 0.25307 factor:1 | 1 (-1.71010) | -1 | -1 |
| G: -5311.84231 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11578.14880 HOMO: -7.06408 LUMO: -2.76196 factor:1 | 1 (-1.94080) | -1 | -1 |
| G: -5311.84231 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11578.33079 HOMO: -5.95657 LUMO: 0.37552 factor:1 | 1 (-2.12279) | -1 | -1 |
| G: -5311.84231 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11578.37721 HOMO: -6.61781 LUMO: 0.02721 factor:1 | 1 (-2.16921) | -1 | -1 |
| G: -5311.84231 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.91239 HOMO: -6.26678 LUMO: -0.66668 factor:1 | 1 (-1.70439) | -1 | -1 |
| G: -5311.84231 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.64634 HOMO: -6.00011 LUMO: -0.13334 factor:1 | 1 (-1.43834) | -1 | -1 |
| G: -5311.84231 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.88866 HOMO: -5.60555 LUMO: 0.67484 factor:1 | 1 (-1.68066) | -1 | -1 |
| G: -5311.84231 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.93949 HOMO: -5.79875 LUMO: 0.99049 factor:1 | 1 (-1.73149) | -1 | -1 |
| G: -5311.84231 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.66830 HOMO: -5.97834 LUMO: 0.48436 factor:1 | 1 (-1.46030) | -1 | -1 |
| G: -5311.84231 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11578.10924 HOMO: -5.82868 LUMO: 0.91974 factor:1 | 1 (-1.90123) | -1 | -1 |
| G: -5311.84231 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11578.33316 HOMO: -5.86677 LUMO: 0.99594 factor:1 | 1 (-2.12515) | -1 | -1 |
| G: -5311.84231 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11578.24845 HOMO: -5.70079 LUMO: 0.48980 factor:1 | 1 (-2.04045) | -1 | -1 |
| G: -5311.84231 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11578.01057 HOMO: -7.39605 LUMO: -1.02315 factor:1 | 1 (-1.80256) | 1 | -1 |
| G: -5311.84231 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.89724 HOMO: -7.22734 LUMO: -1.12927 factor:1 | 1 (-0.68924) | 1 | -1 |
| G: -5311.84231 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.74214 HOMO: -7.58926 LUMO: -0.65035 factor:1 | 1 (-0.53413) | 1 | 1 |
| G: -5311.84231 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.87251 HOMO: -7.43959 LUMO: -0.75648 factor:1 | 1 (-0.66450) | 1 | 1 |
| G: -5311.84231 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.94647 HOMO: -7.55388 LUMO: -1.15104 factor:1 | 1 (-0.73846) | 1 | -1 |
| G: -5311.84231 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.93477 HOMO: -6.74570 LUMO: -2.85447 factor:1 | 1 (-0.72676) | -1 | -1 |
| G: -5311.84231 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.00935 HOMO: -7.35524 LUMO: -1.25444 factor:1 | 1 (-0.80135) | 1 | 1 |
| G: -5311.84231 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.60404 HOMO: -6.81645 LUMO: -1.20819 factor:1 | 1 (-0.39603) | -1 | -1 |
| G: -5311.84231 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.82151 HOMO: -6.99605 LUMO: -1.62996 factor:1 | 1 (-0.61351) | -1 | -1 |
| G: -5311.84231 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.69709 HOMO: -6.88992 LUMO: -0.47620 factor:1 | 1 (-1.48909) | -1 | -1 |
| G: -5311.84231 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11578.51531 HOMO: -7.22190 LUMO: -0.01905 factor:1 | 1 (-2.30731) | 1 | 1 |
| G: -5311.84231 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.89508 HOMO: -6.77836 LUMO: -0.82995 factor:1 | 1 (-1.68708) | -1 | -1 |
| G: -5311.84231 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.93759 HOMO: -6.48447 LUMO: -0.95512 factor:1 | 1 (-1.72958) | -1 | -1 |
| G: -5311.84231 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.63894 HOMO: -7.81239 LUMO: 1.22179 factor:1 | 1 (-1.43094) | 1 | 1 |
| G: -5311.84231 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.71595 HOMO: -7.36612 LUMO: 0.19320 factor:1 | 1 (-1.50795) | 1 | 1 |
| G: -5311.84231 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.60123 HOMO: -7.24095 LUMO: 0.33470 factor:1 | 1 (-1.39322) | 1 | 1 |
| G: -5311.84231 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.75565 HOMO: -7.15932 LUMO: -2.24222 factor:1 | 1 (-1.54765) | -1 | -1 |
| G: -5311.84231 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.65124 HOMO: -6.88992 LUMO: -2.69937 factor:1 | 1 (-1.44324) | -1 | -1 |
| G: -5311.84231 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.98387 HOMO: -6.97428 LUMO: -0.98233 factor:1 | 1 (-1.77587) | -1 | -1 |
| G: -5311.84231 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.89887 HOMO: -7.17564 LUMO: -0.93879 factor:1 | 1 (-0.69087) | 1 | 1 |
| G: -5311.84231 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.09417 HOMO: -6.81645 LUMO: -1.14288 factor:1 | 1 (-0.88617) | -1 | -1 |
| G: -5311.84231 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.98334 HOMO: -6.83006 LUMO: -0.63403 factor:1 | 1 (-0.77533) | -1 | -1 |
| G: -5311.84231 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.03205 HOMO: -7.17292 LUMO: -1.07213 factor:1 | 1 (-0.82404) | 1 | 1 |
| G: -5311.84231 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.01289 HOMO: -7.53755 LUMO: 0.15510 factor:1 | 1 (-0.80489) | 1 | 1 |
| G: -5311.84231 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.98630 HOMO: -6.50080 LUMO: -0.51702 factor:1 | 1 (-0.77830) | -1 | -1 |
| G: -5311.84231 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.23306 HOMO: -6.72665 LUMO: -0.80001 factor:1 | 1 (-1.02505) | -1 | -1 |
| G: -5311.84231 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.17899 HOMO: -6.72665 LUMO: 1.68711 factor:1 | 1 (-0.97098) | -1 | -1 |
| G: -5311.84231 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.77172 HOMO: -7.11850 LUMO: -0.75103 factor:1 | 1 (-0.56371) | 1 | 1 |
| G: -5311.84231 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.86576 HOMO: -6.87087 LUMO: -0.85988 factor:1 | 1 (-0.65775) | -1 | -1 |
| G: -5311.84231 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.77947 HOMO: -7.08857 LUMO: -0.89798 factor:1 | 1 (-0.57147) | 1 | 1 |
| G: -5311.84231 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.99703 HOMO: -6.71305 LUMO: -0.85444 factor:1 | 1 (-0.78902) | -1 | -1 |
| G: -5311.84231 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.72744 HOMO: -6.59332 LUMO: -0.60137 factor:1 | 1 (-0.51944) | -1 | -1 |
| G: -5311.84231 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.03088 HOMO: -7.28993 LUMO: 0.03265 factor:1 | 1 (-0.82287) | 1 | 1 |
| G: -5311.84231 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.98870 HOMO: -7.32258 LUMO: 0.13878 factor:1 | 1 (-0.78069) | 1 | 1 |
| G: -5311.84231 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.95659 HOMO: -7.28993 LUMO: 0.11429 factor:1 | 1 (-0.74859) | 1 | 1 |
| G: -5311.84231 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.06827 HOMO: -6.86271 LUMO: -1.03947 factor:1 | 1 (-0.86026) | -1 | -1 |
| G: -5311.84231 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.91120 HOMO: -6.55794 LUMO: -0.84900 factor:1 | 1 (-0.70320) | -1 | -1 |
| G: -5311.84231 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.25461 HOMO: -7.03686 LUMO: 0.11429 factor:1 | 1 (-1.04660) | -1 | -1 |
| G: -5311.84231 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.89262 HOMO: -7.06952 LUMO: -0.96056 factor:1 | 1 (-0.68461) | 1 | 1 |
| G: -5311.84231 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.63503 HOMO: -6.90897 LUMO: -0.99866 factor:1 | 1 (-0.42703) | -1 | -1 |
| G: -5311.84231 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.90687 HOMO: -7.00693 LUMO: -0.83539 factor:1 | 1 (-0.69887) | -1 | -1 |
| G: -5311.84231 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.69424 HOMO: -6.74298 LUMO: -0.85172 factor:1 | 1 (-0.48624) | -1 | -1 |
| G: -5311.84231 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.97615 HOMO: -6.83822 LUMO: -1.07213 factor:1 | 1 (-0.76815) | -1 | -1 |
| G: -5311.84231 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.05997 HOMO: -7.21918 LUMO: -1.55377 factor:1 | 1 (-0.85196) | 1 | 1 |
| G: -5311.84231 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.75988 HOMO: -6.84094 LUMO: -1.09934 factor:1 | 1 (-0.55187) | -1 | -1 |
| G: -5311.84231 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.98138 HOMO: -7.09129 LUMO: -0.85988 factor:1 | 1 (-0.77337) | 1 | 1 |
| G: -5311.84231 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.89180 HOMO: -6.57971 LUMO: -2.27215 factor:1 | 1 (-0.68379) | -1 | -1 |
| G: -5311.84231 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.85800 HOMO: -6.81373 LUMO: -1.86942 factor:1 | 1 (-0.65000) | -1 | -1 |
| G: -5311.84231 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.76976 HOMO: -6.59060 LUMO: -2.30480 factor:1 | 1 (-0.56175) | -1 | -1 |
| G: -5311.84231 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.49481 HOMO: -6.72938 LUMO: -1.23540 factor:1 | 1 (-0.28681) | -1 | -1 |
| G: -5311.84231 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.62687 HOMO: -6.94707 LUMO: -2.62318 factor:1 | 1 (-0.41886) | -1 | -1 |
| G: -5311.84231 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.54031 HOMO: -7.28177 LUMO: -0.09796 factor:1 | 1 (-0.33231) | 1 | 1 |
| G: -5311.84231 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.89172 HOMO: -6.80013 LUMO: -0.79729 factor:1 | 1 (-0.68371) | -1 | -1 |
| G: -5311.84231 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.98587 HOMO: -7.26544 LUMO: 0.12789 factor:1 | 1 (-0.77786) | 1 | 1 |
| G: -5311.84231 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.88747 HOMO: -6.51713 LUMO: -0.49253 factor:1 | 1 (-0.67947) | -1 | -1 |
| G: -5311.84231 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.07205 HOMO: -6.68856 LUMO: -0.77280 factor:1 | 1 (-0.86404) | -1 | -1 |
| G: -5311.84231 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.73454 HOMO: -6.41100 LUMO: -0.70750 factor:1 | 1 (-0.52654) | -1 | -1 |
| G: -5311.84231 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.13338 HOMO: -7.56204 LUMO: 0.22041 factor:1 | 1 (-0.92538) | 1 | 1 |
| G: -5311.84231 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.00307 HOMO: -6.68312 LUMO: 1.30343 factor:1 | 1 (-0.79506) | -1 | -1 |
| G: -5311.84231 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.07828 HOMO: -7.24367 LUMO: 0.17415 factor:1 | 1 (-0.87027) | 1 | 1 |
| G: -5311.84231 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.34928 HOMO: -7.52395 LUMO: 1.16737 factor:1 | 1 (-1.14127) | 1 | 1 |
| G: -5311.84231 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.16389 HOMO: -6.89264 LUMO: 0.23130 factor:1 | 1 (-0.95588) | -1 | -1 |
| G: -5311.84231 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.98269 HOMO: -7.21102 LUMO: 0.19048 factor:1 | 1 (-0.77468) | 1 | 1 |
| G: -5311.84231 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.92598 HOMO: -7.08312 LUMO: 0.25034 factor:1 | 1 (-0.71797) | 1 | 1 |
| G: -5311.84231 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.99847 HOMO: -6.49536 LUMO: -0.65852 factor:1 | 1 (-0.79046) | -1 | -1 |
| G: -5311.84231 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.17564 HOMO: -6.85455 LUMO: 0.13606 factor:1 | 1 (-0.96764) | -1 | -1 |
| G: -5311.84231 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.10756 HOMO: -7.10217 LUMO: 0.35919 factor:1 | 1 (-0.89955) | 1 | 1 |
| G: -5311.84231 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.14965 HOMO: -7.77429 LUMO: 1.19186 factor:1 | 1 (-0.94165) | 1 | 1 |
| G: -5311.84231 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.28718 HOMO: -6.57427 LUMO: -0.50069 factor:1 | 1 (-1.07918) | -1 | -1 |
| G: -5311.84231 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.83634 HOMO: -7.36340 LUMO: 0.10068 factor:1 | 1 (-0.62834) | 1 | 1 |
| G: -5311.84231 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.87689 HOMO: -7.28177 LUMO: 0.15238 factor:1 | 1 (-0.66888) | 1 | 1 |
| G: -5311.84231 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.76159 HOMO: -6.86543 LUMO: -0.84355 factor:1 | 1 (-0.55359) | -1 | -1 |
| G: -5311.84231 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.96622 HOMO: -6.55794 LUMO: 1.39594 factor:1 | 1 (-0.75822) | -1 | -1 |
| G: -5311.84231 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.91131 HOMO: -6.26134 LUMO: 1.53744 factor:1 | 1 (-0.70331) | -1 | -1 |
| G: -5311.84231 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.75297 HOMO: -5.97562 LUMO: 1.42316 factor:1 | 1 (-0.54496) | -1 | -1 |
| G: -5311.84231 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.09314 HOMO: -6.65046 LUMO: 1.44492 factor:1 | 1 (-0.88513) | -1 | -1 |
| G: -5311.84231 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.01210 HOMO: -6.92258 LUMO: 0.17415 factor:1 | 1 (-0.80410) | -1 | -1 |
| G: -5311.84231 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.00995 HOMO: -7.40966 LUMO: 0.19592 factor:1 | 1 (-0.80195) | 1 | 1 |
| G: -5311.84231 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.68614 HOMO: -7.17564 LUMO: 0.16871 factor:1 | 1 (-0.47813) | 1 | 1 |
| G: -5311.84231 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.64532 HOMO: -7.46953 LUMO: 0.22313 factor:1 | 1 (-0.43731) | 1 | 1 |
| G: -5311.84231 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.46450 HOMO: -6.13345 LUMO: 1.85854 factor:1 | 1 (-0.25649) | -1 | -1 |
| G: -5311.84231 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.57027 HOMO: -6.99333 LUMO: -1.65717 factor:1 | 1 (-0.36227) | -1 | -1 |
| G: -5311.84231 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.93199 HOMO: -6.93074 LUMO: -1.79323 factor:1 | 1 (-0.72399) | -1 | -1 |
| G: -5311.84231 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.86516 HOMO: -6.87904 LUMO: -1.79323 factor:1 | 1 (-0.65715) | -1 | -1 |
| G: -5311.84231 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.87806 HOMO: -6.84094 LUMO: 0.66940 factor:1 | 1 (-0.67005) | -1 | -1 |
| G: -5311.84231 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.01920 HOMO: -7.13210 LUMO: -1.17553 factor:1 | 1 (-0.81120) | 1 | 1 |
| G: -5311.84231 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.99382 HOMO: -6.52801 LUMO: -2.23678 factor:1 | 1 (-0.78581) | -1 | -1 |
| G: -5311.84231 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.21148 HOMO: -6.81917 LUMO: -1.86398 factor:1 | 1 (-1.00347) | -1 | -1 |
| G: -5311.84231 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.05012 HOMO: -7.30626 LUMO: -1.66806 factor:1 | 1 (-0.84211) | 1 | 1 |
| G: -5311.84231 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.05969 HOMO: -6.98516 LUMO: -1.40683 factor:1 | 1 (-0.85169) | -1 | -1 |
| G: -5311.84231 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.91713 HOMO: -6.95523 LUMO: -0.97145 factor:1 | 1 (-0.70913) | -1 | -1 |
| G: -5311.84231 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.74649 HOMO: -6.83278 LUMO: -2.68848 factor:1 | 1 (-0.53849) | -1 | -1 |
| G: -5311.84231 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.71291 HOMO: -7.25456 LUMO: -2.97420 factor:1 | 1 (-0.50491) | -1 | -1 |
| G: -5311.84231 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.62253 HOMO: -6.80557 LUMO: -2.65039 factor:1 | 1 (-1.41453) | -1 | -1 |
| G: -5311.84231 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.46533 HOMO: -7.10489 LUMO: 0.77008 factor:1 | 1 (-1.25733) | 1 | -1 |
| G: -5311.84231 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.58476 HOMO: -7.28993 LUMO: -1.06124 factor:1 | 1 (-1.37676) | 1 | 1 |
| G: -5311.84231 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.75299 HOMO: -7.11578 LUMO: -1.10206 factor:1 | 1 (-1.54498) | 1 | 1 |
| G: -5311.84231 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.85318 HOMO: -6.91713 LUMO: -1.36329 factor:1 | 1 (-1.64517) | -1 | -1 |
| G: -5311.84231 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.64346 HOMO: -7.07224 LUMO: 0.51974 factor:1 | 1 (-1.43546) | 1 | 1 |
| G: -5311.84231 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.48506 HOMO: -7.22734 LUMO: -0.93335 factor:1 | 1 (-1.27706) | 1 | 1 |
| G: -5311.84231 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.33309 HOMO: -7.19469 LUMO: -0.96600 factor:1 | 1 (-1.12508) | 1 | 1 |
| G: -5311.84231 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.73184 HOMO: -6.93890 LUMO: -0.66940 factor:1 | 1 (-1.52384) | -1 | -1 |
| G: -5311.84231 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11578.19977 HOMO: -7.09673 LUMO: -1.05852 factor:1 | 1 (-1.99176) | 1 | 1 |
| G: -5311.84231 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11578.08622 HOMO: -7.19197 LUMO: -2.26943 factor:1 | 1 (-1.87821) | -1 | -1 |
| G: -5311.84231 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11578.23781 HOMO: -6.90081 LUMO: -2.64767 factor:1 | 1 (-2.02981) | -1 | -1 |
| G: -5311.84231 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11578.80296 HOMO: -6.93890 LUMO: -2.65039 factor:1 | 1 (-2.59496) | -1 | -1 |
| G: -5311.84231 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11579.10817 HOMO: -6.80013 LUMO: -2.54154 factor:1 | 1 (-2.90016) | -1 | -1 |
| G: -5311.84231 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11578.32276 HOMO: -6.68040 LUMO: -0.89798 factor:1 | 1 (-2.11476) | -1 | -1 |
| G: -5311.84231 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.77533 HOMO: -7.01782 LUMO: -1.09662 factor:1 | 1 (-1.56732) | -1 | -1 |
| G: -5311.84231 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.98591 HOMO: -6.58516 LUMO: -0.83539 factor:1 | 1 (-1.77791) | -1 | -1 |
| G: -5311.84231 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.87840 HOMO: -7.46953 LUMO: 0.06259 factor:1 | 1 (-1.67040) | 1 | 1 |
| G: -5311.84231 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.97277 HOMO: -6.96884 LUMO: -0.99866 factor:1 | 1 (-1.76477) | -1 | -1 |
| G: -5311.84231 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.69840 HOMO: -7.29809 LUMO: -0.19320 factor:1 | 1 (-1.49039) | 1 | 1 |
| G: -5311.84231 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.94856 HOMO: -6.86271 LUMO: 0.04082 factor:1 | 1 (-0.74056) | -1 | -1 |
| G: -5311.84231 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.87166 HOMO: -6.36746 LUMO: -1.02587 factor:1 | 1 (-0.66366) | -1 | -1 |
| G: -5311.84231 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.90965 HOMO: -7.15659 LUMO: -1.25989 factor:1 | 1 (-0.70165) | 1 | 1 |
| G: -5311.84231 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.00655 HOMO: -6.69128 LUMO: -0.59865 factor:1 | 1 (-0.79855) | -1 | -1 |
| G: -5311.84231 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.11714 HOMO: -7.09129 LUMO: -1.08573 factor:1 | 1 (-0.90913) | 1 | 1 |
| G: -5311.84231 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.12220 HOMO: -6.64502 LUMO: -0.66396 factor:1 | 1 (-0.91419) | -1 | -1 |
| G: -5311.84231 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.85648 HOMO: -6.93346 LUMO: -0.87349 factor:1 | 1 (-0.64847) | -1 | -1 |
| G: -5311.84231 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.81740 HOMO: -6.77019 LUMO: -0.87349 factor:1 | 1 (-0.60940) | -1 | -1 |
| G: -5311.84231 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.81618 HOMO: -6.59060 LUMO: -0.82995 factor:1 | 1 (-0.60817) | -1 | -1 |
| G: -5311.84231 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.95885 HOMO: -7.17564 LUMO: -1.08846 factor:1 | 1 (-0.75084) | 1 | 1 |
| G: -5311.84231 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.83052 HOMO: -7.27088 LUMO: -1.18642 factor:1 | 1 (-0.62251) | 1 | 1 |
| G: -5311.84231 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.01050 HOMO: -7.06680 LUMO: -1.13199 factor:1 | 1 (-0.80249) | 1 | 1 |
| G: -5311.84231 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.80295 HOMO: -7.21918 LUMO: -1.03947 factor:1 | 1 (-0.59495) | 1 | 1 |
| G: -5311.84231 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.01471 HOMO: -7.26000 LUMO: -0.11973 factor:1 | 1 (-0.80671) | 1 | 1 |
| G: -5311.84231 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.19855 HOMO: -6.77564 LUMO: 0.23402 factor:1 | 1 (-0.99055) | -1 | -1 |
| G: -5311.84231 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.72736 HOMO: -7.07224 LUMO: -0.75648 factor:1 | 1 (-0.51936) | 1 | 1 |
| G: -5311.84231 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.88973 HOMO: -7.45048 LUMO: 0.18232 factor:1 | 1 (-0.68173) | 1 | 1 |
| G: -5311.84231 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.88704 HOMO: -7.48313 LUMO: 0.15238 factor:1 | 1 (-0.67903) | 1 | 1 |
| G: -5311.84231 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.73245 HOMO: -6.60692 LUMO: -0.50885 factor:1 | 1 (-0.52445) | -1 | -1 |
| G: -5311.84231 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.97768 HOMO: -6.62869 LUMO: -0.60954 factor:1 | 1 (-0.76967) | -1 | -1 |
| G: -5311.84231 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.81076 HOMO: -7.40422 LUMO: -1.28982 factor:1 | 1 (-0.60276) | 1 | 1 |
| G: -5311.84231 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.05297 HOMO: -6.75114 LUMO: -1.23268 factor:1 | 1 (-0.84497) | -1 | -1 |
| G: -5311.84231 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.90119 HOMO: -6.84638 LUMO: -0.73199 factor:1 | 1 (-0.69318) | -1 | -1 |
| G: -5311.84231 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.74421 HOMO: -6.79196 LUMO: -1.43676 factor:1 | 1 (-0.53620) | -1 | -1 |
| G: -5311.84231 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.64317 HOMO: -7.00965 LUMO: -1.37690 factor:1 | 1 (-0.43516) | -1 | -1 |
| G: -5311.84231 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.00709 HOMO: -6.97972 LUMO: -1.58098 factor:1 | 1 (-0.79909) | -1 | -1 |
| G: -5311.84231 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11578.18804 HOMO: -6.91169 LUMO: -1.48574 factor:1 | 1 (-1.98004) | -1 | -1 |
| G: -5311.84231 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11578.94767 HOMO: -6.90081 LUMO: -1.30343 factor:1 | 1 (-2.73967) | -1 | -1 |
| G: -5311.84231 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11578.05460 HOMO: -6.78652 LUMO: -1.51840 factor:1 | 1 (-1.84659) | -1 | -1 |
| G: -5311.84231 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11578.37251 HOMO: -6.84638 LUMO: -1.15104 factor:1 | 1 (-2.16450) | -1 | -1 |
| G: -5311.84231 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11578.11675 HOMO: -6.61237 LUMO: -0.89798 factor:1 | 1 (-1.90874) | -1 | -1 |
| G: -5311.84231 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.80815 HOMO: -7.16204 LUMO: -1.30070 factor:1 | 1 (-0.60015) | 1 | 1 |
| G: -5311.84231 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.66565 HOMO: -7.32803 LUMO: 0.14694 factor:1 | 1 (-0.45764) | 1 | 1 |
| G: -5311.84231 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.82271 HOMO: -6.99877 LUMO: -0.87621 factor:1 | 1 (-0.61471) | -1 | -1 |
| G: -5311.84231 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.76521 HOMO: -6.99877 LUMO: -0.97145 factor:1 | 1 (-0.55721) | -1 | -1 |
| G: -5311.84231 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.98837 HOMO: -7.08040 LUMO: -1.09662 factor:1 | 1 (-0.78037) | 1 | 1 |
| G: -5311.84231 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.71746 HOMO: -6.90897 LUMO: -1.14016 factor:1 | 1 (-0.50945) | -1 | -1 |
| G: -5311.84231 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.72151 HOMO: -6.68312 LUMO: -0.74831 factor:1 | 1 (-0.51351) | -1 | -1 |
| G: -5311.84231 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.47764 HOMO: -6.99061 LUMO: -0.86804 factor:1 | 1 (-0.26964) | -1 | -1 |
| G: -5311.84231 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.97221 HOMO: -7.10761 LUMO: -1.18642 factor:1 | 1 (-0.76420) | 1 | 1 |
| G: -5311.84231 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.79710 HOMO: -6.79196 LUMO: -0.71294 factor:1 | 1 (-1.58909) | -1 | -1 |
| G: -5311.84231 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11578.39194 HOMO: -6.86271 LUMO: -0.81362 factor:1 | 1 (-2.18393) | -1 | -1 |
| G: -5311.84231 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.66313 HOMO: -7.01510 LUMO: -0.99322 factor:1 | 1 (-1.45513) | -1 | -1 |
| G: -5311.84231 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.80635 HOMO: -6.88720 LUMO: -0.87893 factor:1 | 1 (-1.59834) | -1 | -1 |
| G: -5311.84231 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.96902 HOMO: -6.88448 LUMO: 0.22041 factor:1 | 1 (-1.76101) | -1 | -1 |
| G: -5311.84231 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.70898 HOMO: -7.55932 LUMO: 1.12111 factor:1 | 1 (-1.50098) | 1 | 1 |
| G: -5311.84231 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.65320 HOMO: -6.46815 LUMO: -0.86260 factor:1 | 1 (-1.44520) | -1 | -1 |
| G: -5311.84231 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.97879 HOMO: -7.13755 LUMO: 0.23130 factor:1 | 1 (-1.77078) | 1 | 1 |
| G: -5311.84231 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.60357 HOMO: -6.78924 LUMO: 1.51023 factor:1 | 1 (-1.39556) | -1 | -1 |
| G: -5311.84231 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.78003 HOMO: -6.48992 LUMO: 1.74969 factor:1 | 1 (-1.57203) | -1 | -1 |
| G: -5311.84231 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.99318 HOMO: -6.78380 LUMO: 1.81500 factor:1 | 1 (-1.78518) | -1 | -1 |
| G: -5311.84231 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.89133 HOMO: -6.49536 LUMO: 1.70615 factor:1 | 1 (-1.68332) | -1 | -1 |
| G: -5311.84231 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.64357 HOMO: -6.38651 LUMO: 1.44492 factor:1 | 1 (-1.43556) | -1 | -1 |
| G: -5311.84231 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.71337 HOMO: -6.83822 LUMO: 1.38234 factor:1 | 1 (-1.50536) | -1 | -1 |
| G: -5311.84231 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.56610 HOMO: -6.01644 LUMO: 1.20274 factor:1 | 1 (-1.35809) | -1 | -1 |
| G: -5311.84231 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11578.20581 HOMO: -6.18243 LUMO: 1.77962 factor:1 | 1 (-1.99781) | -1 | -1 |
| G: -5311.84231 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11578.78011 HOMO: -6.81917 LUMO: -1.01771 factor:1 | 1 (-2.57210) | -1 | -1 |
| G: -5311.84231 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11578.16317 HOMO: -6.61237 LUMO: -0.91702 factor:1 | 1 (-1.95517) | -1 | -1 |
| G: -5311.84231 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.93772 HOMO: -6.84094 LUMO: -0.84900 factor:1 | 1 (-1.72972) | -1 | -1 |
| G: -5311.84231 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.96855 HOMO: -6.81917 LUMO: -1.01771 factor:1 | 1 (-1.76055) | -1 | -1 |
| G: -5311.84231 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.74956 HOMO: -7.86953 LUMO: 1.16737 factor:1 | 1 (-1.54155) | 1 | 1 |
| G: -5311.84231 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.61415 HOMO: -7.40694 LUMO: 0.11429 factor:1 | 1 (-1.40615) | 1 | 1 |
| G: -5311.84231 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.65117 HOMO: -6.70489 LUMO: -0.65035 factor:1 | 1 (-0.44316) | -1 | -1 |
| G: -5311.84231 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.87381 HOMO: -7.23279 LUMO: 0.33470 factor:1 | 1 (-0.66581) | 1 | 1 |
| G: -5311.84231 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.86274 HOMO: -7.17020 LUMO: 0.41361 factor:1 | 1 (-0.65473) | 1 | 1 |
| G: -5311.84231 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.77433 HOMO: -6.90353 LUMO: -0.90070 factor:1 | 1 (-0.56632) | -1 | -1 |
| G: -5311.84231 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.75863 HOMO: -7.39061 LUMO: 0.17687 factor:1 | 1 (-0.55062) | 1 | 1 |
| G: -5311.84231 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.69073 HOMO: -7.16748 LUMO: 0.42178 factor:1 | 1 (-0.48273) | 1 | 1 |
| G: -5311.84231 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.88622 HOMO: -7.36884 LUMO: -1.11295 factor:1 | 1 (-0.67822) | 1 | 1 |
| G: -5311.84231 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.68766 HOMO: -7.33347 LUMO: 0.33198 factor:1 | 1 (-0.47966) | 1 | 1 |
| G: -5311.84231 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.96815 HOMO: -7.31986 LUMO: -0.83539 factor:1 | 1 (-0.76015) | 1 | 1 |
| G: -5311.84231 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.72434 HOMO: -7.31170 LUMO: 0.08708 factor:1 | 1 (-0.51634) | 1 | 1 |
| G: -5311.84231 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.81936 HOMO: -7.36884 LUMO: 0.38096 factor:1 | 1 (-0.61136) | 1 | 1 |
| G: -5311.84231 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.56866 HOMO: -6.99333 LUMO: 1.74153 factor:1 | 1 (-0.36066) | -1 | -1 |
| G: -5311.84231 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.96481 HOMO: -6.94435 LUMO: 1.74969 factor:1 | 1 (-0.75680) | -1 | -1 |
| G: -5311.84231 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.69520 HOMO: -7.02598 LUMO: 1.43404 factor:1 | 1 (-0.48719) | -1 | -1 |
| G: -5311.84231 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.60766 HOMO: -6.41100 LUMO: 1.62996 factor:1 | 1 (-0.39965) | -1 | -1 |
| G: -5311.84231 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.55049 HOMO: -6.57699 LUMO: 1.81228 factor:1 | 1 (-0.34248) | -1 | -1 |
| G: -5311.84231 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.70728 HOMO: -6.86543 LUMO: 1.49935 factor:1 | 1 (-0.49927) | -1 | -1 |
| G: -5311.84231 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.79612 HOMO: -6.91169 LUMO: -1.22451 factor:1 | 1 (-0.58812) | -1 | -1 |
| G: -5311.84231 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11578.01846 HOMO: -7.09945 LUMO: -1.23812 factor:1 | 1 (-1.81046) | 1 | 1 |
| G: -5311.84231 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11579.11029 HOMO: -7.48857 LUMO: 0.10340 factor:1 | 1 (-2.90228) | 1 | 1 |
| G: -5311.84231 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11578.18981 HOMO: -7.21918 LUMO: -0.06803 factor:1 | 1 (-1.98181) | 1 | 1 |
| G: -5311.84231 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.64992 HOMO: -6.34025 LUMO: -0.68845 factor:1 | 1 (-0.44191) | -1 | -1 |
| G: -5311.84231 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.78140 HOMO: -6.82734 LUMO: -0.77825 factor:1 | 1 (-0.57340) | -1 | -1 |
| G: -5311.84231 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.79923 HOMO: -6.92258 LUMO: -1.03675 factor:1 | 1 (-0.59122) | -1 | -1 |
| G: -5311.84231 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.64826 HOMO: -6.42461 LUMO: -0.95240 factor:1 | 1 (-0.44025) | -1 | -1 |
| G: -5311.84231 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.81841 HOMO: -6.96067 LUMO: -1.05036 factor:1 | 1 (-0.61041) | -1 | -1 |
| G: -5311.84231 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11578.35662 HOMO: -7.23551 LUMO: 0.12245 factor:1 | 1 (-2.14861) | 1 | 1 |
| G: -5311.84231 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.73696 HOMO: -6.85183 LUMO: 0.16055 factor:1 | 1 (-1.52895) | -1 | -1 |
| G: -5311.84231 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.65111 HOMO: -6.46815 LUMO: -0.89253 factor:1 | 1 (-1.44310) | -1 | -1 |
| G: -5311.84231 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.76719 HOMO: -7.23823 LUMO: -0.06259 factor:1 | 1 (-1.55919) | 1 | 1 |
| G: -5311.84231 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.73451 HOMO: -6.76475 LUMO: -0.99049 factor:1 | 1 (-1.52650) | -1 | -1 |
| G: -5311.84231 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.85348 HOMO: -7.14843 LUMO: -0.88165 factor:1 | 1 (-1.64547) | 1 | 1 |
| G: -5311.84231 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11578.54348 HOMO: -7.15659 LUMO: 0.20681 factor:1 | 1 (-2.33547) | 1 | 1 |
| G: -5311.84231 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.61078 HOMO: -7.11306 LUMO: 0.14150 factor:1 | 1 (-1.40277) | 1 | 1 |
| G: -5311.84231 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.94834 HOMO: -6.67223 LUMO: -0.86260 factor:1 | 1 (-0.74034) | -1 | -1 |
| G: -5311.84231 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.11657 HOMO: -6.92530 LUMO: 0.30749 factor:1 | 1 (-0.90856) | -1 | -1 |
| G: -5311.84231 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.05782 HOMO: -6.50624 LUMO: -0.70477 factor:1 | 1 (-0.84981) | -1 | -1 |
| G: -5311.84231 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.05474 HOMO: -7.35524 LUMO: 0.75103 factor:1 | 1 (-0.84674) | 1 | 1 |
| G: -5311.84231 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.01033 HOMO: -7.07768 LUMO: -0.26939 factor:1 | 1 (-0.80233) | 1 | 1 |
| G: -5311.84231 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.11205 HOMO: -7.15932 LUMO: 0.42450 factor:1 | 1 (-0.90404) | 1 | 1 |
| G: -5311.84231 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.89569 HOMO: -7.46136 LUMO: 0.04626 factor:1 | 1 (-0.68769) | 1 | 1 |
| G: -5311.84231 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.76061 HOMO: -7.05047 LUMO: -1.06669 factor:1 | 1 (-0.55261) | -1 | -1 |
| G: -5311.84231 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.28996 HOMO: -6.66951 LUMO: -0.99322 factor:1 | 1 (-1.08195) | -1 | -1 |
| G: -5311.84231 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.12642 HOMO: -7.01782 LUMO: -1.08846 factor:1 | 1 (-0.91841) | -1 | -1 |
| G: -5311.84231 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.16683 HOMO: -7.03959 LUMO: -1.15376 factor:1 | 1 (-0.95882) | -1 | -1 |
| G: -5311.84231 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.12282 HOMO: -6.68856 LUMO: 1.61364 factor:1 | 1 (-0.91482) | -1 | -1 |
| G: -5311.84231 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.26968 HOMO: -6.53345 LUMO: 1.60275 factor:1 | 1 (-1.06168) | -1 | -1 |
| G: -5311.84231 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.27975 HOMO: -6.73482 LUMO: 1.86398 factor:1 | 1 (-1.07175) | -1 | -1 |
| G: -5311.84231 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.99694 HOMO: -6.87632 LUMO: 1.59731 factor:1 | 1 (-0.78894) | -1 | -1 |
| G: -5311.84231 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.02563 HOMO: -6.31848 LUMO: 2.12521 factor:1 | 1 (-0.81762) | -1 | -1 |
| G: -5311.84231 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.49426 HOMO: -6.35114 LUMO: 1.71432 factor:1 | 1 (-1.28626) | -1 | -1 |
| G: -5311.84231 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.27080 HOMO: -6.34842 LUMO: 1.92929 factor:1 | 1 (-1.06280) | -1 | -1 |
| G: -5311.84231 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.21970 HOMO: -6.14977 LUMO: 1.78235 factor:1 | 1 (-1.01169) | -1 | -1 |
| G: -5311.84231 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.41154 HOMO: -6.31032 LUMO: 1.51567 factor:1 | 1 (-1.20353) | -1 | -1 |
| G: -5311.84231 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.12786 HOMO: -6.25862 LUMO: 1.75241 factor:1 | 1 (-0.91985) | -1 | -1 |
| G: -5311.84231 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.03646 HOMO: -6.49264 LUMO: 1.66806 factor:1 | 1 (-0.82845) | -1 | -1 |
| G: -5311.84231 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.04252 HOMO: -6.28311 LUMO: 1.60003 factor:1 | 1 (-0.83452) | -1 | -1 |
| G: -5311.84231 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.17208 HOMO: -7.13210 LUMO: -0.04354 factor:1 | 1 (-0.96407) | 1 | 1 |
| G: -5311.84231 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.27534 HOMO: -7.35252 LUMO: 0.03537 factor:1 | 1 (-1.06734) | 1 | 1 |
| G: -5311.84231 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.19602 HOMO: -6.58243 LUMO: -0.48980 factor:1 | 1 (-0.98802) | -1 | -1 |
| G: -5311.84231 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.34925 HOMO: -6.90081 LUMO: -0.05442 factor:1 | 1 (-1.14125) | -1 | -1 |
| G: -5311.84231 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.23695 HOMO: -7.22734 LUMO: 0.17143 factor:1 | 1 (-1.02894) | 1 | 1 |
| G: -5311.84231 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.24002 HOMO: -7.13210 LUMO: -0.99866 factor:1 | 1 (-1.03202) | 1 | 1 |
| G: -5311.84231 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.05303 HOMO: -7.39878 LUMO: 0.13334 factor:1 | 1 (-0.84502) | 1 | 1 |
| G: -5311.84231 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.00054 HOMO: -7.04503 LUMO: -0.89798 factor:1 | 1 (-0.79253) | -1 | -1 |
| G: -5311.84231 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.78951 HOMO: -6.95523 LUMO: -1.07213 factor:1 | 1 (-0.58151) | -1 | -1 |
| G: -5311.84231 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.03101 HOMO: -6.75114 LUMO: -1.28438 factor:1 | 1 (-0.82301) | -1 | -1 |
| G: -5311.84231 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.20609 HOMO: -6.75114 LUMO: -0.11701 factor:1 | 1 (-0.99809) | -1 | -1 |
| G: -5311.84231 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.03836 HOMO: -6.83278 LUMO: -0.01633 factor:1 | 1 (-0.83036) | -1 | -1 |
| G: -5311.84231 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.91520 HOMO: -6.93890 LUMO: -0.88981 factor:1 | 1 (-0.70720) | -1 | -1 |
| G: -5311.84231 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.18606 HOMO: -7.07224 LUMO: -1.08573 factor:1 | 1 (-0.97806) | 1 | 1 |
| G: -5311.84231 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.73112 HOMO: -6.99877 LUMO: -0.95240 factor:1 | 1 (-0.52311) | -1 | -1 |
| G: -5311.84231 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.61925 HOMO: -7.09129 LUMO: 0.35375 factor:1 | 1 (-0.41125) | 1 | 1 |
| G: -5311.84231 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.08764 HOMO: -7.09401 LUMO: 0.04354 factor:1 | 1 (-0.87964) | 1 | 1 |
| G: -5311.84231 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.22753 HOMO: -6.85183 LUMO: -0.68573 factor:1 | 1 (-1.01953) | -1 | -1 |
| G: -5311.84231 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.01792 HOMO: -6.83006 LUMO: -0.58777 factor:1 | 1 (-0.80992) | -1 | -1 |
| G: -5311.84231 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.30457 HOMO: -7.40422 LUMO: 0.17687 factor:1 | 1 (-1.09656) | 1 | 1 |
| G: -5311.84231 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.11387 HOMO: -7.15932 LUMO: 0.10340 factor:1 | 1 (-0.90587) | 1 | 1 |
| G: -5311.84231 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.87577 HOMO: -7.03414 LUMO: -0.19592 factor:1 | 1 (-0.66777) | -1 | -1 |
| G: -5311.84231 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.67611 HOMO: -6.48447 LUMO: -0.36191 factor:1 | 1 (-1.46811) | -1 | -1 |
| G: -5311.84231 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.67802 HOMO: -7.49402 LUMO: 0.11429 factor:1 | 1 (-1.47001) | 1 | 1 |
| G: -5311.84231 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.99155 HOMO: -7.01237 LUMO: -1.06397 factor:1 | 1 (-1.78354) | -1 | -1 |
| G: -5311.84231 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.90575 HOMO: -6.67223 LUMO: -1.07213 factor:1 | 1 (-1.69775) | -1 | -1 |
| G: -5311.84231 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.85865 HOMO: -7.38789 LUMO: -1.15376 factor:1 | 1 (-1.65064) | 1 | 1 |
| G: -5311.84231 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.81416 HOMO: -6.42461 LUMO: -1.23812 factor:1 | 1 (-1.60615) | -1 | -1 |
| G: -5311.84231 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11578.01541 HOMO: -7.36884 LUMO: -1.19186 factor:1 | 1 (-1.80741) | 1 | 1 |
| G: -5311.84231 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11578.09452 HOMO: -6.65591 LUMO: 0.07075 factor:1 | 1 (-1.88651) | -1 | -1 |
| G: -5311.84231 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.90474 HOMO: -7.39061 LUMO: -0.16871 factor:1 | 1 (-1.69674) | 1 | 1 |
| G: -5311.84231 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.85944 HOMO: -6.90353 LUMO: -0.96056 factor:1 | 1 (-1.65143) | -1 | -1 |
| G: -5311.84231 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.87750 HOMO: -7.42054 LUMO: 0.19048 factor:1 | 1 (-1.66950) | 1 | 1 |
| G: -5311.84231 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.94532 HOMO: -7.40150 LUMO: 0.35647 factor:1 | 1 (-1.73731) | 1 | 1 |
| G: -5311.84231 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.53225 HOMO: -6.56067 LUMO: -0.96056 factor:1 | 1 (-1.32424) | -1 | -1 |
| G: -5311.84231 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.52909 HOMO: -6.89809 LUMO: -0.81090 factor:1 | 1 (-1.32109) | -1 | -1 |
| G: -5311.84231 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.18925 HOMO: -6.91986 LUMO: -0.84900 factor:1 | 1 (-0.98124) | -1 | -1 |
| G: -5311.84231 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.09014 HOMO: -6.61509 LUMO: -0.62042 factor:1 | 1 (-0.88214) | -1 | -1 |
| G: -5311.84231 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.02601 HOMO: -6.58243 LUMO: -0.65579 factor:1 | 1 (-0.81800) | -1 | -1 |
| G: -5311.84231 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.12761 HOMO: -6.52257 LUMO: -0.92519 factor:1 | 1 (-0.91961) | -1 | -1 |
| G: -5311.84231 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.23515 HOMO: -6.69128 LUMO: 1.49118 factor:1 | 1 (-1.02715) | -1 | -1 |
| G: -5311.84231 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.42912 HOMO: -7.02870 LUMO: 1.67894 factor:1 | 1 (-1.22111) | -1 | -1 |
| G: -5311.84231 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.25564 HOMO: -6.88720 LUMO: 1.68711 factor:1 | 1 (-1.04764) | -1 | -1 |
| G: -5311.84231 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.07262 HOMO: -5.89943 LUMO: 1.03675 factor:1 | 1 (-0.86461) | -1 | -1 |
| G: -5311.84231 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.96851 HOMO: -6.40556 LUMO: 1.14560 factor:1 | 1 (-0.76050) | -1 | -1 |
| G: -5311.84231 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.64830 HOMO: -6.51168 LUMO: 1.48030 factor:1 | 1 (-1.44030) | -1 | -1 |
| G: -5311.84231 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.78792 HOMO: -6.64502 LUMO: 1.91568 factor:1 | 1 (-1.57992) | -1 | -1 |
| G: -5311.84231 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.77935 HOMO: -6.47903 LUMO: 1.91296 factor:1 | 1 (-1.57135) | -1 | -1 |
| G: -5311.84231 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.48000 HOMO: -6.34297 LUMO: 1.91840 factor:1 | 1 (-1.27200) | -1 | -1 |
| G: -5311.84231 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.60520 HOMO: -6.89809 LUMO: 1.82861 factor:1 | 1 (-1.39720) | -1 | -1 |
| G: -5311.84231 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.52966 HOMO: -6.10079 LUMO: 1.62996 factor:1 | 1 (-1.32166) | -1 | -1 |
| G: -5311.84231 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.73465 HOMO: -7.16476 LUMO: -0.92247 factor:1 | 1 (-1.52664) | 1 | 1 |
| G: -5311.84231 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.79674 HOMO: -7.10489 LUMO: -0.95784 factor:1 | 1 (-1.58874) | 1 | 1 |
| G: -5311.84231 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.89661 HOMO: -6.76475 LUMO: -0.99866 factor:1 | 1 (-1.68860) | -1 | -1 |
| G: -5311.84231 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.76188 HOMO: -6.81373 LUMO: -1.05036 factor:1 | 1 (-1.55388) | -1 | -1 |
| G: -5311.84231 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.63121 HOMO: -6.90081 LUMO: -1.03947 factor:1 | 1 (-1.42321) | -1 | -1 |
| G: -5311.84231 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.66942 HOMO: -7.06952 LUMO: -0.91702 factor:1 | 1 (-1.46141) | 1 | 1 |
| G: -5311.84231 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.44680 HOMO: -6.73482 LUMO: -0.94151 factor:1 | 1 (-1.23880) | -1 | -1 |
| G: -5311.84231 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.38041 HOMO: -6.99605 LUMO: -1.04764 factor:1 | 1 (-1.17240) | -1 | -1 |
| G: -5311.84231 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.87582 HOMO: -7.03686 LUMO: -0.93335 factor:1 | 1 (-1.66781) | -1 | -1 |
| G: -5311.84231 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.78741 HOMO: -6.81101 LUMO: -0.95240 factor:1 | 1 (-1.57940) | -1 | -1 |
| G: -5311.84231 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.57883 HOMO: -6.83822 LUMO: -0.65307 factor:1 | 1 (-1.37083) | -1 | -1 |
| G: -5311.84231 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.53548 HOMO: -7.05319 LUMO: -0.81634 factor:1 | 1 (-1.32748) | -1 | -1 |
| G: -5311.84231 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.71884 HOMO: -7.57565 LUMO: 0.19048 factor:1 | 1 (-1.51083) | 1 | 1 |
| G: -5311.84231 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.56027 HOMO: -6.56067 LUMO: -0.50613 factor:1 | 1 (-1.35227) | -1 | -1 |
| G: -5311.84231 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.60539 HOMO: -6.74298 LUMO: -0.70477 factor:1 | 1 (-1.39739) | -1 | -1 |
| G: -5311.84231 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.86542 HOMO: -7.02054 LUMO: 0.03537 factor:1 | 1 (-1.65742) | -1 | -1 |
| G: -5311.84231 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.84153 HOMO: -7.33347 LUMO: -0.17960 factor:1 | 1 (-1.63353) | 1 | 1 |
| G: -5311.84231 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.79122 HOMO: -6.98244 LUMO: -0.88165 factor:1 | 1 (-1.58321) | -1 | -1 |
| G: -5311.84231 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.86757 HOMO: -7.14843 LUMO: -1.19730 factor:1 | 1 (-1.65957) | 1 | 1 |
| G: -5311.84231 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.44610 HOMO: -7.17564 LUMO: -1.21907 factor:1 | 1 (-1.23809) | 1 | 1 |
| G: -5311.84231 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.48253 HOMO: -6.74026 LUMO: -0.86532 factor:1 | 1 (-1.27453) | -1 | -1 |
| G: -5311.84231 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11578.00534 HOMO: -6.82462 LUMO: -1.24084 factor:1 | 1 (-1.79734) | -1 | -1 |
| G: -5311.84231 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.02437 HOMO: -6.78924 LUMO: -0.70477 factor:1 | 1 (-0.81637) | -1 | -1 |
| G: -5311.84231 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.83112 HOMO: -7.41238 LUMO: 0.05987 factor:1 | 1 (-0.62311) | 1 | 1 |
| G: -5311.84231 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.03741 HOMO: -6.75931 LUMO: 0.02721 factor:1 | 1 (-0.82940) | -1 | -1 |
| G: -5311.84231 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.16111 HOMO: -6.28583 LUMO: -0.93063 factor:1 | 1 (-0.95311) | -1 | -1 |
| G: -5311.84231 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.77963 HOMO: -6.69128 LUMO: -0.83539 factor:1 | 1 (-0.57163) | -1 | -1 |
| G: -5311.84231 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.97368 HOMO: -7.22190 LUMO: 0.01361 factor:1 | 1 (-0.76567) | 1 | 1 |
| G: -5311.84231 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.91398 HOMO: -6.95251 LUMO: -1.09934 factor:1 | 1 (-0.70597) | -1 | -1 |
| G: -5311.84231 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.86132 HOMO: -6.75387 LUMO: -0.90614 factor:1 | 1 (-0.65332) | -1 | -1 |
| G: -5311.84231 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.74589 HOMO: -7.48585 LUMO: 0.05987 factor:1 | 1 (-0.53789) | 1 | 1 |
| G: -5311.84231 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.68246 HOMO: -6.92802 LUMO: -0.66940 factor:1 | 1 (-0.47446) | -1 | -1 |
| G: -5311.84231 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.05036 HOMO: -7.29537 LUMO: -0.14150 factor:1 | 1 (-0.84236) | 1 | 1 |
| G: -5311.84231 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.90026 HOMO: -6.57155 LUMO: -0.86804 factor:1 | 1 (-0.69226) | -1 | -1 |
| G: -5311.84231 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.29856 HOMO: -6.87632 LUMO: -0.77825 factor:1 | 1 (-1.09055) | -1 | -1 |
| G: -5311.84231 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.01833 HOMO: -6.45998 LUMO: -0.31565 factor:1 | 1 (-0.81033) | -1 | -1 |
| G: -5311.84231 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.92728 HOMO: -7.51306 LUMO: 0.05714 factor:1 | 1 (-0.71928) | 1 | 1 |
| G: -5311.84231 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.89828 HOMO: -6.86271 LUMO: -0.00816 factor:1 | 1 (-0.69027) | -1 | -1 |
| G: -5311.84231 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.85180 HOMO: -6.43277 LUMO: -1.07485 factor:1 | 1 (-0.64379) | -1 | -1 |
| G: -5311.84231 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.98070 HOMO: -6.78108 LUMO: -0.81362 factor:1 | 1 (-0.77269) | -1 | -1 |
| G: -5311.84231 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.20810 HOMO: -6.88448 LUMO: 1.21907 factor:1 | 1 (-1.00010) | -1 | -1 |
| G: -5311.84231 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.69237 HOMO: -6.97700 LUMO: 1.44765 factor:1 | 1 (-0.48436) | -1 | -1 |
| G: -5311.84231 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.96824 HOMO: -6.89537 LUMO: 2.12249 factor:1 | 1 (-0.76023) | -1 | -1 |
| G: -5311.84231 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.09997 HOMO: -6.28311 LUMO: 1.45037 factor:1 | 1 (-0.89196) | -1 | -1 |
| G: -5311.84231 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.91844 HOMO: -6.55522 LUMO: 1.39867 factor:1 | 1 (-0.71043) | -1 | -1 |
| G: -5311.84231 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.90443 HOMO: -6.46815 LUMO: 1.50207 factor:1 | 1 (-0.69642) | -1 | -1 |
| G: -5311.84231 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.82214 HOMO: -6.43549 LUMO: 2.17419 factor:1 | 1 (-0.61413) | -1 | -1 |
| G: -5311.84231 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.06573 HOMO: -6.99333 LUMO: 1.87214 factor:1 | 1 (-0.85773) | -1 | -1 |
| G: -5311.84231 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.81558 HOMO: -6.65591 LUMO: 1.37962 factor:1 | 1 (-0.60758) | -1 | -1 |
| G: -5311.84231 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.76570 HOMO: -6.82734 LUMO: 1.55649 factor:1 | 1 (-0.55770) | -1 | -1 |
| G: -5311.84231 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.68400 HOMO: -6.71849 LUMO: 1.36057 factor:1 | 1 (-1.47600) | -1 | -1 |
| G: -5311.84231 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.88300 HOMO: -6.79468 LUMO: 1.82044 factor:1 | 1 (-1.67500) | -1 | -1 |
| G: -5311.84231 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.80422 HOMO: -6.61237 LUMO: 1.15104 factor:1 | 1 (-1.59622) | -1 | -1 |
| G: -5311.84231 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.33064 HOMO: -6.62053 LUMO: 2.33474 factor:1 | 1 (-1.12263) | -1 | -1 |
| G: -5311.84231 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.75894 HOMO: -6.55794 LUMO: 1.65717 factor:1 | 1 (-1.55094) | -1 | -1 |
| G: -5311.84231 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.47532 HOMO: -6.85999 LUMO: 2.03813 factor:1 | 1 (-1.26732) | -1 | -1 |
| G: -5311.84231 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.45513 HOMO: -6.45726 LUMO: 1.28438 factor:1 | 1 (-1.24713) | -1 | -1 |
| G: -5311.84231 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.65290 HOMO: -6.23685 LUMO: 1.93201 factor:1 | 1 (-1.44490) | -1 | -1 |
| G: -5311.84231 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.93150 HOMO: -7.06680 LUMO: 1.86942 factor:1 | 1 (-0.72350) | 1 | 1 |
| G: -5311.84231 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.92059 HOMO: -6.89537 LUMO: 2.17147 factor:1 | 1 (-0.71258) | -1 | -1 |
| G: -5311.84231 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.20541 HOMO: -6.80013 LUMO: 1.78779 factor:1 | 1 (-0.99741) | -1 | -1 |
| G: -5311.84231 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.73593 HOMO: -6.45726 LUMO: 1.58370 factor:1 | 1 (-0.52793) | -1 | -1 |
| G: -5311.84231 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.74094 HOMO: -6.52529 LUMO: 1.71976 factor:1 | 1 (-0.53293) | -1 | -1 |
| G: -5311.84231 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.04489 HOMO: -7.22462 LUMO: -1.18642 factor:1 | 1 (-0.83689) | 1 | 1 |
| G: -5311.84231 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.92568 HOMO: -7.18381 LUMO: -0.78641 factor:1 | 1 (-0.71767) | 1 | 1 |
| G: -5311.84231 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.98187 HOMO: -6.93346 LUMO: 1.65717 factor:1 | 1 (-0.77386) | -1 | -1 |
| G: -5311.84231 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.27722 HOMO: -6.41644 LUMO: 1.78235 factor:1 | 1 (-1.06922) | -1 | -1 |
| G: -5311.84231 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.82358 HOMO: -6.59876 LUMO: 1.83677 factor:1 | 1 (-0.61558) | -1 | -1 |
| G: -5311.84231 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.57054 HOMO: -6.35658 LUMO: 1.59731 factor:1 | 1 (-0.36254) | -1 | -1 |
| G: -5311.84231 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.08184 HOMO: -6.60692 LUMO: 1.66534 factor:1 | 1 (-0.87384) | -1 | -1 |
| G: -5311.84231 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.70129 HOMO: -6.83006 LUMO: 2.11705 factor:1 | 1 (-0.49329) | -1 | -1 |
| G: -5311.84231 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.94511 HOMO: -6.89264 LUMO: 1.30070 factor:1 | 1 (-0.73710) | -1 | -1 |
| G: -5311.84231 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.06628 HOMO: -6.90081 LUMO: 2.05174 factor:1 | 1 (-0.85827) | -1 | -1 |
| G: -5311.84231 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.78309 HOMO: -6.74842 LUMO: 1.96194 factor:1 | 1 (-0.57509) | -1 | -1 |
| G: -5311.84231 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.83762 HOMO: -6.58516 LUMO: 1.30887 factor:1 | 1 (-0.62962) | -1 | -1 |
| G: -5311.84231 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.66676 HOMO: -7.00965 LUMO: 2.08167 factor:1 | 1 (-0.45876) | -1 | -1 |
| G: -5311.84231 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.03112 HOMO: -6.86815 LUMO: 2.29664 factor:1 | 1 (-0.82312) | -1 | -1 |
| G: -5311.84231 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.22819 HOMO: -6.39740 LUMO: 2.02725 factor:1 | 1 (-1.02018) | -1 | -1 |
| G: -5311.84231 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.85466 HOMO: -5.95929 LUMO: 1.62724 factor:1 | 1 (-0.64665) | -1 | -1 |
| G: -5311.84231 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.01031 HOMO: -6.71849 LUMO: 1.34696 factor:1 | 1 (-0.80230) | -1 | -1 |
| G: -5311.84231 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.97088 HOMO: -7.26816 LUMO: 1.74153 factor:1 | 1 (-0.76287) | 1 | 1 |
| G: -5311.84231 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.19308 HOMO: -6.90897 LUMO: 1.71432 factor:1 | 1 (-0.98508) | -1 | -1 |
| G: -5311.84231 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.08269 HOMO: -6.70489 LUMO: 1.91568 factor:1 | 1 (-0.87468) | -1 | -1 |
| G: -5311.84231 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.92135 HOMO: -6.83278 LUMO: 1.61908 factor:1 | 1 (-0.71335) | -1 | -1 |
| G: -5311.84231 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.92456 HOMO: -7.17292 LUMO: 1.95378 factor:1 | 1 (-0.71656) | 1 | -1 |
| G: -5311.84231 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.84701 HOMO: -6.53345 LUMO: 1.74153 factor:1 | 1 (-0.63900) | -1 | -1 |
| G: -5311.84231 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.89330 HOMO: -6.53073 LUMO: 1.51023 factor:1 | 1 (-0.68529) | -1 | -1 |
| G: -5311.84231 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.72197 HOMO: -6.93346 LUMO: 2.22861 factor:1 | 1 (-0.51397) | -1 | -1 |
| G: -5311.84231 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.94451 HOMO: -6.47903 LUMO: 2.05446 factor:1 | 1 (-0.73650) | -1 | -1 |
| G: -5311.84231 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.79626 HOMO: -6.88992 LUMO: 1.57010 factor:1 | 1 (-0.58826) | -1 | -1 |
| G: -5311.84231 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.07939 HOMO: -6.07358 LUMO: 1.95922 factor:1 | 1 (-0.87139) | -1 | -1 |
| G: -5311.84231 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.96478 HOMO: -6.75114 LUMO: 2.18780 factor:1 | 1 (-0.75678) | -1 | -1 |
| G: -5311.84231 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.76636 HOMO: -6.96339 LUMO: 1.70071 factor:1 | 1 (-0.55835) | -1 | -1 |
| G: -5311.84231 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.13714 HOMO: -7.14843 LUMO: 1.82588 factor:1 | 1 (-0.92913) | 1 | -1 |
| G: -5311.84231 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.75381 HOMO: -6.96339 LUMO: 2.29392 factor:1 | 1 (-0.54581) | -1 | -1 |
| G: -5311.84231 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.68619 HOMO: -6.81645 LUMO: 2.39732 factor:1 | 1 (-0.47819) | -1 | -1 |
| G: -5311.84231 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.49944 HOMO: -6.48447 LUMO: 1.24084 factor:1 | 1 (-0.29143) | -1 | -1 |
| G: -5311.84231 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.92116 HOMO: -7.14843 LUMO: 2.01092 factor:1 | 1 (-0.71316) | 1 | -1 |
| G: -5311.84231 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.03504 HOMO: -7.20013 LUMO: -0.34286 factor:1 | 1 (-0.82704) | 1 | -1 |
| G: -5311.84231 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.07667 HOMO: -6.97700 LUMO: -0.15238 factor:1 | 1 (-0.86867) | -1 | -1 |
| G: -5311.84231 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.74293 HOMO: -7.07768 LUMO: -0.26123 factor:1 | 1 (-0.53492) | 1 | -1 |
| G: -5311.84231 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.64899 HOMO: -6.99333 LUMO: -0.41361 factor:1 | 1 (-0.44099) | -1 | -1 |
| G: -5311.84231 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.11213 HOMO: -6.84638 LUMO: -0.40273 factor:1 | 1 (-0.90413) | -1 | -1 |
| G: -5311.84231 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.13232 HOMO: -6.83822 LUMO: -0.26939 factor:1 | 1 (-0.92432) | -1 | -1 |
| G: -5311.84231 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.21714 HOMO: -6.75931 LUMO: -0.93879 factor:1 | 1 (-1.00913) | -1 | -1 |
| G: -5311.84231 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.27488 HOMO: -6.79468 LUMO: -0.39729 factor:1 | 1 (-1.06688) | -1 | -1 |
| G: -5311.84231 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.01229 HOMO: -6.93890 LUMO: 0.43266 factor:1 | 1 (-0.80429) | -1 | -1 |
| G: -5311.84231 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.12990 HOMO: -7.08040 LUMO: -0.85716 factor:1 | 1 (-0.92189) | 1 | 1 |
| G: -5311.84231 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.98062 HOMO: -6.70216 LUMO: -1.41499 factor:1 | 1 (-0.77261) | -1 | -1 |
| G: -5311.84231 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.63745 HOMO: -6.63686 LUMO: -0.52790 factor:1 | 1 (-1.42944) | -1 | -1 |
| G: -5311.84231 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.52874 HOMO: -6.75114 LUMO: -0.13334 factor:1 | 1 (-1.32073) | -1 | -1 |
| G: -5311.84231 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.70515 HOMO: -6.94435 LUMO: -0.24490 factor:1 | 1 (-1.49714) | -1 | -1 |
| G: -5311.84231 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.89748 HOMO: -6.74298 LUMO: -0.84627 factor:1 | 1 (-1.68947) | -1 | -1 |
| G: -5311.84231 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.57842 HOMO: -7.15932 LUMO: 0.22041 factor:1 | 1 (-1.37042) | 1 | 1 |
| G: -5311.84231 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.45472 HOMO: -6.90081 LUMO: -1.16737 factor:1 | 1 (-1.24672) | -1 | -1 |
| G: -5311.84231 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.96644 HOMO: -7.04775 LUMO: -0.84355 factor:1 | 1 (-0.75844) | -1 | -1 |
| G: -5311.84231 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.98712 HOMO: -7.17020 LUMO: -1.31159 factor:1 | 1 (-0.77912) | 1 | 1 |
| G: -5311.84231 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.79120 HOMO: -7.14571 LUMO: -0.46259 factor:1 | 1 (-0.58319) | 1 | 1 |
| G: -5311.84231 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.68412 HOMO: -7.45048 LUMO: -0.91158 factor:1 | 1 (-0.47612) | 1 | 1 |
| G: -5311.84231 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.41359 HOMO: -6.87360 LUMO: -0.82995 factor:1 | 1 (-0.20558) | -1 | -1 |
| G: -5311.84231 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.86970 HOMO: -7.43415 LUMO: -0.65307 factor:1 | 1 (-0.66170) | 1 | 1 |
| G: -5311.84231 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.60431 HOMO: -7.47225 LUMO: -0.77280 factor:1 | 1 (-0.39631) | 1 | 1 |
| G: -5311.84231 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.29957 HOMO: -6.86271 LUMO: -0.83811 factor:1 | 1 (-0.09157) | -1 | -1 |
| G: -5311.84231 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.16326 HOMO: -7.53483 LUMO: -0.66124 factor:1 | 1 (-0.95526) | 1 | 1 |
| G: -5311.84231 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.08745 HOMO: -7.45864 LUMO: -1.08301 factor:1 | 1 (-0.87944) | 1 | 1 |
| G: -5311.84231 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.26451 HOMO: -7.24639 LUMO: -1.19186 factor:1 | 1 (-1.05651) | 1 | 1 |
| G: -5311.84231 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.38332 HOMO: -7.54844 LUMO: -0.96873 factor:1 | 1 (-1.17531) | 1 | 1 |
| G: -5311.84231 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.39948 HOMO: -7.12666 LUMO: -0.01633 factor:1 | 1 (-1.19148) | 1 | 1 |
| G: -5311.84231 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.03632 HOMO: -6.77291 LUMO: -0.70477 factor:1 | 1 (-0.82831) | -1 | -1 |
| G: -5311.84231 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.09812 HOMO: -6.76475 LUMO: -1.15921 factor:1 | 1 (-0.89011) | -1 | -1 |
| G: -5311.84231 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.94685 HOMO: -5.37697 LUMO: -0.56600 factor:1 | 1 (-0.73884) | -1 | -1 |
| G: -5311.84231 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.28601 HOMO: -6.62053 LUMO: -1.75513 factor:1 | 1 (-1.07801) | -1 | -1 |
| G: -5311.84231 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.99713 HOMO: -6.60420 LUMO: -1.74697 factor:1 | 1 (-0.78913) | -1 | -1 |
| G: -5311.84231 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.09074 HOMO: -6.84366 LUMO: -0.94968 factor:1 | 1 (-0.88274) | -1 | -1 |
| G: -5311.84231 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.34656 HOMO: -6.96884 LUMO: -2.11977 factor:1 | 1 (-1.13855) | -1 | -1 |
| G: -5311.84231 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.19115 HOMO: -6.80829 LUMO: 0.56055 factor:1 | 1 (-0.98315) | -1 | -1 |
| G: -5311.84231 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.84086 HOMO: -7.02326 LUMO: 0.11429 factor:1 | 1 (-0.63286) | -1 | -1 |
| G: -5311.84231 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.68709 HOMO: -7.40966 LUMO: 0.18232 factor:1 | 1 (-0.47908) | 1 | 1 |
| G: -5311.84231 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.80132 HOMO: -6.34570 LUMO: 0.41089 factor:1 | 1 (-0.59332) | -1 | -1 |
| G: -5311.84231 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.69625 HOMO: -6.78924 LUMO: 0.49525 factor:1 | 1 (-1.48825) | -1 | -1 |
| G: -5311.84231 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.81827 HOMO: -6.87632 LUMO: 0.44082 factor:1 | 1 (-1.61026) | -1 | -1 |
| G: -5311.84231 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.88526 HOMO: -6.69944 LUMO: 1.20546 factor:1 | 1 (-1.67726) | -1 | -1 |
| G: -5311.84231 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.88980 HOMO: -6.83006 LUMO: 1.28982 factor:1 | 1 (-1.68180) | -1 | -1 |
| G: -5311.84231 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11578.06652 HOMO: -7.78246 LUMO: 0.20681 factor:1 | 1 (-1.85851) | 1 | 1 |
| G: -5311.84231 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.83829 HOMO: -6.55794 LUMO: -1.65173 factor:1 | 1 (-1.63029) | -1 | -1 |
| G: -5311.84231 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.65535 HOMO: -6.77564 LUMO: -1.14560 factor:1 | 1 (-1.44735) | -1 | -1 |
| G: -5311.84231 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.04835 HOMO: -7.46680 LUMO: -1.18097 factor:1 | 1 (-0.84034) | 1 | 1 |
| G: -5311.84231 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.15640 HOMO: -6.88176 LUMO: -1.24900 factor:1 | 1 (-0.94840) | -1 | -1 |
| G: -5311.84231 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.17488 HOMO: -7.28177 LUMO: -0.42178 factor:1 | 1 (-0.96687) | 1 | 1 |
| G: -5311.84231 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.31189 HOMO: -7.71715 LUMO: 0.19592 factor:1 | 1 (-1.10388) | 1 | 1 |
| G: -5311.84231 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.35012 HOMO: -7.02326 LUMO: -1.40683 factor:1 | 1 (-1.14212) | -1 | -1 |
| G: -5311.84231 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.09091 HOMO: -7.27088 LUMO: -1.07485 factor:1 | 1 (-0.88290) | 1 | 1 |
| G: -5311.84231 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.99406 HOMO: -7.17020 LUMO: -0.49525 factor:1 | 1 (-0.78606) | 1 | 1 |
| G: -5311.84231 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.75104 HOMO: -7.15932 LUMO: 0.02721 factor:1 | 1 (-0.54303) | 1 | 1 |
| G: -5311.84231 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.06114 HOMO: -7.00693 LUMO: -0.83267 factor:1 | 1 (-0.85313) | -1 | -1 |
| G: -5311.84231 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.94192 HOMO: -6.86543 LUMO: -0.10340 factor:1 | 1 (-0.73392) | -1 | -1 |
| G: -5311.84231 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.88837 HOMO: -7.11850 LUMO: -0.08980 factor:1 | 1 (-0.68037) | 1 | 1 |
| G: -5311.84231 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.07659 HOMO: -6.87087 LUMO: -0.88981 factor:1 | 1 (-0.86859) | -1 | -1 |
| G: -5311.84231 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.91991 HOMO: -7.08857 LUMO: -1.27077 factor:1 | 1 (-0.71190) | 1 | 1 |
| G: -5311.84231 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.06304 HOMO: -6.79468 LUMO: -0.81906 factor:1 | 1 (-0.85504) | -1 | -1 |
| G: -5311.84231 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.96138 HOMO: -6.86815 LUMO: -0.89798 factor:1 | 1 (-0.75337) | -1 | -1 |
| G: -5311.84231 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.70750 HOMO: -6.78652 LUMO: -2.00548 factor:1 | 1 (-0.49949) | -1 | -1 |
| G: -5311.84231 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.84739 HOMO: -6.75114 LUMO: -0.08436 factor:1 | 1 (-0.63939) | -1 | -1 |
| G: -5311.84231 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.58676 HOMO: -6.55794 LUMO: 0.52790 factor:1 | 1 (-0.37876) | -1 | -1 |
| G: -5311.84231 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.81666 HOMO: -7.17836 LUMO: 0.28300 factor:1 | 1 (-1.60866) | 1 | -1 |
| G: -5311.84231 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.73437 HOMO: -7.35796 LUMO: -0.77552 factor:1 | 1 (-1.52637) | 1 | 1 |
| G: -5311.84231 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.79914 HOMO: -7.23551 LUMO: -1.17553 factor:1 | 1 (-1.59113) | 1 | 1 |
| G: -5311.84231 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.63399 HOMO: -7.07496 LUMO: -1.14288 factor:1 | 1 (-1.42599) | 1 | 1 |
| G: -5311.84231 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.89179 HOMO: -6.70489 LUMO: -0.83539 factor:1 | 1 (-1.68379) | -1 | -1 |
| G: -5311.84231 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.87125 HOMO: -6.59604 LUMO: -0.89798 factor:1 | 1 (-1.66324) | -1 | -1 |
| G: -5311.84231 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11578.06064 HOMO: -6.94162 LUMO: -1.22451 factor:1 | 1 (-1.85263) | -1 | -1 |
| G: -5311.84231 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.61208 HOMO: -6.68040 LUMO: 0.22041 factor:1 | 1 (-1.40408) | -1 | -1 |
| G: -5311.84231 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.62373 HOMO: -6.88176 LUMO: 0.11157 factor:1 | 1 (-1.41573) | -1 | -1 |
| G: -5311.84231 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.53227 HOMO: -6.91713 LUMO: 1.27621 factor:1 | 1 (-1.32427) | -1 | -1 |
| G: -5311.84231 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.94232 HOMO: -6.77836 LUMO: 1.01226 factor:1 | 1 (-1.73432) | -1 | -1 |
| G: -5311.84231 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.12125 HOMO: -7.14571 LUMO: 1.48574 factor:1 | 1 (-0.91324) | 1 | 1 |
| G: -5311.84231 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.03354 HOMO: -6.96884 LUMO: 1.48574 factor:1 | 1 (-0.82554) | -1 | -1 |
| G: -5311.84231 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.34838 HOMO: -7.24367 LUMO: 1.28438 factor:1 | 1 (-1.14037) | 1 | 1 |
| G: -5311.84231 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.90081 HOMO: -7.10489 LUMO: 1.29526 factor:1 | 1 (-0.69280) | 1 | 1 |
| G: -5311.84231 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.73860 HOMO: -7.07224 LUMO: 1.29254 factor:1 | 1 (-0.53059) | 1 | 1 |
| G: -5311.84231 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.93972 HOMO: -7.12938 LUMO: 0.49253 factor:1 | 1 (-0.73171) | 1 | 1 |
| G: -5311.84231 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.95477 HOMO: -7.33619 LUMO: 1.45581 factor:1 | 1 (-0.74676) | 1 | 1 |
| G: -5311.84231 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.23238 HOMO: -6.87904 LUMO: -0.14422 factor:1 | 1 (-1.02437) | -1 | -1 |
| G: -5311.84231 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.09940 HOMO: -6.81917 LUMO: 0.50341 factor:1 | 1 (-0.89139) | -1 | -1 |
| G: -5311.84231 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.70935 HOMO: -7.27905 LUMO: 0.13606 factor:1 | 1 (-0.50134) | 1 | -1 |
| G: -5311.84231 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.63765 HOMO: -6.87904 LUMO: -0.09796 factor:1 | 1 (-0.42964) | -1 | -1 |
| G: -5311.84231 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.10530 HOMO: -7.33891 LUMO: 0.03810 factor:1 | 1 (-0.89730) | 1 | 1 |
| G: -5311.84231 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.99441 HOMO: -6.98516 LUMO: 0.98233 factor:1 | 1 (-0.78641) | -1 | -1 |
| G: -5311.84231 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.93267 HOMO: -6.94162 LUMO: 0.86804 factor:1 | 1 (-0.72467) | -1 | -1 |
| G: -5311.84231 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.20152 HOMO: -7.37701 LUMO: 0.05442 factor:1 | 1 (-0.99351) | 1 | 1 |
| G: -5311.84231 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.25621 HOMO: -7.04775 LUMO: 0.43266 factor:1 | 1 (-1.04821) | -1 | -1 |
| G: -5311.84231 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.79329 HOMO: -7.47497 LUMO: 0.31837 factor:1 | 1 (-0.58529) | 1 | 1 |
| G: -5311.84231 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.80742 HOMO: -6.62053 LUMO: 0.13061 factor:1 | 1 (-0.59941) | -1 | -1 |
| G: -5311.84231 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.01920 HOMO: -6.44366 LUMO: -0.04354 factor:1 | 1 (-0.81120) | -1 | -1 |
| G: -5311.84231 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.68891 HOMO: -6.40284 LUMO: 0.68301 factor:1 | 1 (-0.48091) | -1 | -1 |
| G: -5311.84231 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.49084 HOMO: -6.73754 LUMO: 0.36735 factor:1 | 1 (-0.28284) | -1 | -1 |
| G: -5311.84231 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.67669 HOMO: -6.85455 LUMO: 0.23946 factor:1 | 1 (-0.46869) | -1 | -1 |
| G: -5311.84231 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.59922 HOMO: -6.93346 LUMO: 0.24762 factor:1 | 1 (-0.39122) | -1 | -1 |
| G: -5311.84231 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.93433 HOMO: -6.85455 LUMO: 0.17687 factor:1 | 1 (-0.72633) | -1 | -1 |
| G: -5311.84231 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.64290 HOMO: -6.62325 LUMO: 0.69933 factor:1 | 1 (-0.43489) | -1 | -1 |
| G: -5311.84231 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.13787 HOMO: -6.43005 LUMO: 0.50069 factor:1 | 1 (-0.92987) | -1 | -1 |
| G: -5311.84231 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.85610 HOMO: -6.56883 LUMO: 0.22858 factor:1 | 1 (-0.64809) | -1 | -1 |
| G: -5311.84231 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.02211 HOMO: -6.78380 LUMO: 0.54967 factor:1 | 1 (-0.81411) | -1 | -1 |
| G: -5311.84231 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.09765 HOMO: -7.35524 LUMO: 0.00272 factor:1 | 1 (-0.88965) | 1 | 1 |
| G: -5311.84231 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.72420 HOMO: -7.27360 LUMO: 0.08436 factor:1 | 1 (-0.51620) | 1 | 1 |
| G: -5311.84231 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.97920 HOMO: -7.44504 LUMO: -0.96056 factor:1 | 1 (-0.77120) | 1 | 1 |
| G: -5311.84231 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.78480 HOMO: -7.27360 LUMO: 0.29933 factor:1 | 1 (-0.57680) | 1 | 1 |
| G: -5311.84231 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.86992 HOMO: -7.09129 LUMO: 0.41089 factor:1 | 1 (-0.66192) | 1 | 1 |
| G: -5311.84231 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.14786 HOMO: -6.93618 LUMO: 0.36463 factor:1 | 1 (-0.93985) | -1 | -1 |
| G: -5311.84231 HOMO: -7.26000 LUMO: -3.02863 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.73572 HOMO: -7.65728 LUMO: 0.20136 factor:1 | 1 (-0.52771) | 1 | 1 |
| G: -5311.84231 HOMO: -7.26000 LUMO: -3.02863 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.45800 HOMO: -6.90353 LUMO: -0.92791 factor:1 | 1 (-0.24999) | -1 | -1 |
| G: -5311.84231 HOMO: -7.26000 LUMO: -3.02863 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.77854 HOMO: -6.82462 LUMO: -1.18370 factor:1 | 1 (-1.57053) | -1 | -1 |
| G: -5311.84231 HOMO: -7.26000 LUMO: -3.02863 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.95933 HOMO: -7.09129 LUMO: -0.13334 factor:1 | 1 (-1.75132) | 1 | 1 |
| G: -5311.84231 HOMO: -7.26000 LUMO: -3.02863 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.75620 HOMO: -7.40966 LUMO: -1.06941 factor:1 | 1 (-1.54819) | 1 | 1 |
| G: -5311.84231 HOMO: -7.26000 LUMO: -3.02863 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.81748 HOMO: -7.24367 LUMO: -1.00954 factor:1 | 1 (-1.60947) | 1 | 1 |
| G: -5311.84231 HOMO: -7.26000 LUMO: -3.02863 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.87786 HOMO: -7.51851 LUMO: 0.09796 factor:1 | 1 (-1.66985) | 1 | 1 |
| G: -5311.84231 HOMO: -7.26000 LUMO: -3.02863 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11578.09582 HOMO: -7.48857 LUMO: -0.07619 factor:1 | 1 (-1.88782) | 1 | 1 |
| G: -5311.84231 HOMO: -7.26000 LUMO: -3.02863 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11578.06219 HOMO: -6.53345 LUMO: 1.09390 factor:1 | 1 (-1.85418) | -1 | -1 |
| G: -5311.84231 HOMO: -7.26000 LUMO: -3.02863 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.79258 HOMO: -7.21918 LUMO: 0.08436 factor:1 | 1 (-1.58457) | 1 | 1 |
| G: -5311.84231 HOMO: -7.26000 LUMO: -3.02863 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.97930 HOMO: -7.38789 LUMO: 1.02587 factor:1 | 1 (-1.77130) | 1 | -1 |
| G: -5311.84231 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.65464 HOMO: -6.83550 LUMO: -0.67484 factor:1 | 1 (-1.44664) | -1 | -1 |
| G: -5311.84231 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.59236 HOMO: -7.04231 LUMO: 0.54151 factor:1 | 1 (-1.38435) | -1 | -1 |
| G: -5311.84231 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.58583 HOMO: -6.79740 LUMO: 1.91296 factor:1 | 1 (-1.37782) | 1 | 1 |
| G: -5311.84231 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.70866 HOMO: -7.35796 LUMO: -1.04220 factor:1 | 1 (-1.50065) | -1 | -1 |
| G: -5311.84231 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.61007 HOMO: -6.62597 LUMO: -0.44082 factor:1 | 1 (-1.40207) | -1 | -1 |
| G: -5311.84231 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.45736 HOMO: -6.45182 LUMO: -0.20409 factor:1 | 1 (-1.24936) | -1 | -1 |
| G: -5311.84231 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.84159 HOMO: -6.51168 LUMO: -0.23130 factor:1 | 1 (-1.63358) | -1 | -1 |
| G: -5311.84231 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.73775 HOMO: -7.14027 LUMO: 0.49797 factor:1 | 1 (-1.52974) | -1 | -1 |
| G: -5311.84231 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.76866 HOMO: -7.55660 LUMO: 0.24762 factor:1 | 1 (-1.56065) | -1 | -1 |
| G: -5311.84231 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.69198 HOMO: -6.88992 LUMO: -0.64763 factor:1 | 1 (-1.48397) | -1 | -1 |
| G: -5311.84231 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.64398 HOMO: -6.72665 LUMO: -0.45987 factor:1 | 1 (-1.43597) | -1 | -1 |
| G: -5311.84231 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.45382 HOMO: -6.72121 LUMO: -0.58232 factor:1 | 1 (-1.24582) | -1 | -1 |
| G: -5311.84231 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.45067 HOMO: -7.26816 LUMO: 0.32926 factor:1 | 1 (-1.24266) | -1 | -1 |
| G: -5311.84231 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.73813 HOMO: -6.57155 LUMO: -0.53606 factor:1 | 1 (-1.53012) | -1 | -1 |
| G: -5311.84231 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.61706 HOMO: -6.50896 LUMO: -0.43810 factor:1 | 1 (-1.40906) | -1 | -1 |
| G: -5311.84231 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.77612 HOMO: -6.73210 LUMO: -0.51430 factor:1 | 1 (-1.56811) | -1 | -1 |
| G: -5311.84231 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.90036 HOMO: -6.77019 LUMO: -0.62858 factor:1 | 1 (-1.69236) | -1 | -1 |
| G: -5311.84231 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.63804 HOMO: -6.82462 LUMO: -0.67484 factor:1 | 1 (-1.43004) | -1 | -1 |
| G: -5311.84231 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.69415 HOMO: -6.79740 LUMO: -0.55511 factor:1 | 1 (-1.48615) | -1 | -1 |
| G: -5311.84231 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.90746 HOMO: -6.79740 LUMO: -0.67756 factor:1 | 1 (-1.69946) | -1 | -1 |
| G: -5311.84231 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.72390 HOMO: -6.75114 LUMO: -0.55239 factor:1 | 1 (-1.51589) | -1 | -1 |
| G: -5311.84231 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.56887 HOMO: -6.49536 LUMO: -0.25307 factor:1 | 1 (-1.36087) | -1 | -1 |
| G: -5311.84231 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.67791 HOMO: -6.48992 LUMO: -0.25034 factor:1 | 1 (-1.46990) | -1 | -1 |
| G: -5311.84231 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.82305 HOMO: -6.52801 LUMO: -0.28028 factor:1 | 1 (-1.61505) | -1 | -1 |
| G: -5311.84231 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.67788 HOMO: -7.22462 LUMO: 0.52518 factor:1 | 1 (-1.46988) | -1 | -1 |
| G: -5311.84231 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.51148 HOMO: -6.59332 LUMO: -0.27211 factor:1 | 1 (-1.30348) | -1 | -1 |
| G: -5311.84231 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.85220 HOMO: -6.57427 LUMO: -0.16871 factor:1 | 1 (-1.64419) | -1 | -1 |
| G: -5311.84231 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.90191 HOMO: -6.71033 LUMO: 1.59187 factor:1 | 1 (-1.69391) | 1 | 1 |
| G: -5311.84231 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.75690 HOMO: -6.72121 LUMO: 2.00004 factor:1 | 1 (-1.54890) | 1 | 1 |
| G: -5311.84231 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.96763 HOMO: -6.61509 LUMO: 1.55921 factor:1 | 1 (-1.75962) | -1 | -1 |
| G: -5311.84231 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.71554 HOMO: -6.55250 LUMO: 1.73064 factor:1 | 1 (-1.50754) | -1 | -1 |
| G: -5311.84231 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.29466 HOMO: -6.66135 LUMO: 2.02181 factor:1 | 1 (-1.08666) | 1 | 1 |
| G: -5311.84231 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.44297 HOMO: -6.84911 LUMO: 1.98099 factor:1 | 1 (-1.23496) | 1 | 1 |
| G: -5311.84231 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.58400 HOMO: -6.66679 LUMO: 1.98371 factor:1 | 1 (-1.37600) | 1 | 1 |
| G: -5311.84231 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.84418 HOMO: -6.67495 LUMO: 2.04085 factor:1 | 1 (-0.63617) | 1 | 1 |
| G: -5311.84231 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.94143 HOMO: -6.89809 LUMO: 1.95106 factor:1 | 1 (-0.73343) | 1 | 1 |
| G: -5311.84231 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.01006 HOMO: -6.50352 LUMO: 1.88847 factor:1 | 1 (-0.80206) | -1 | -1 |
| G: -5311.84231 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.90769 HOMO: -6.93618 LUMO: 2.00004 factor:1 | 1 (-0.69969) | 1 | 1 |
| G: -5311.84231 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.05496 HOMO: -6.50896 LUMO: 1.73609 factor:1 | 1 (-0.84695) | -1 | -1 |
| G: -5311.84231 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.99221 HOMO: -6.69672 LUMO: 2.37283 factor:1 | 1 (-0.78420) | 1 | 1 |
| G: -5311.84231 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.17472 HOMO: -6.65591 LUMO: 2.20684 factor:1 | 1 (-0.96671) | 1 | 1 |
| G: -5311.84231 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.13744 HOMO: -6.23957 LUMO: 1.78507 factor:1 | 1 (-0.92943) | -1 | -1 |
| G: -5311.84231 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.99251 HOMO: -6.35114 LUMO: 1.92112 factor:1 | 1 (-0.78450) | -1 | -1 |
| G: -5311.84231 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.84116 HOMO: -6.53617 LUMO: 1.75241 factor:1 | 1 (-0.63315) | -1 | -1 |
| G: -5311.84231 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.16936 HOMO: -6.60420 LUMO: 1.78779 factor:1 | 1 (-0.96135) | 1 | 1 |
| G: -5311.84231 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.78358 HOMO: -7.40422 LUMO: -0.97145 factor:1 | 1 (-0.57558) | -1 | -1 |
| G: -5311.84231 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.80780 HOMO: -6.80013 LUMO: -0.69117 factor:1 | 1 (-0.59979) | -1 | -1 |
| G: -5311.84231 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.70978 HOMO: -6.68040 LUMO: -0.47076 factor:1 | 1 (-0.50178) | -1 | -1 |
| G: -5311.84231 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.79713 HOMO: -7.20285 LUMO: -0.66124 factor:1 | 1 (-0.58913) | -1 | -1 |
| G: -5311.84231 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.78929 HOMO: -6.82734 LUMO: -0.60137 factor:1 | 1 (-0.58129) | -1 | -1 |
| G: -5311.84231 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.94217 HOMO: -7.18653 LUMO: 0.59321 factor:1 | 1 (-0.73416) | -1 | -1 |
| G: -5311.84231 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.12008 HOMO: -7.29265 LUMO: 0.48164 factor:1 | 1 (-0.91207) | -1 | -1 |
| G: -5311.84231 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.01882 HOMO: -6.63414 LUMO: -0.25034 factor:1 | 1 (-0.81082) | -1 | -1 |
| G: -5311.84231 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.95409 HOMO: -7.20285 LUMO: 0.53879 factor:1 | 1 (-0.74608) | -1 | -1 |
| G: -5311.84231 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.79112 HOMO: -6.46815 LUMO: -0.21769 factor:1 | 1 (-0.58311) | -1 | -1 |
| G: -5311.84231 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.77260 HOMO: -6.57971 LUMO: -0.18776 factor:1 | 1 (-1.56460) | -1 | -1 |
| G: -5311.84231 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.95446 HOMO: -6.90897 LUMO: 1.91296 factor:1 | 1 (-1.74645) | 1 | 1 |
| G: -5311.84231 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.84308 HOMO: -6.67495 LUMO: 2.04358 factor:1 | 1 (-1.63508) | 1 | 1 |
| G: -5311.84231 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.64814 HOMO: -6.94162 LUMO: 1.73881 factor:1 | 1 (-1.44014) | 1 | 1 |
| G: -5311.84231 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.96434 HOMO: -6.73482 LUMO: 1.95922 factor:1 | 1 (-1.75633) | 1 | 1 |
| G: -5311.84231 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.87887 HOMO: -6.70489 LUMO: 2.04358 factor:1 | 1 (-1.67086) | 1 | 1 |
| G: -5311.84231 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11578.05479 HOMO: -7.04231 LUMO: 1.79323 factor:1 | 1 (-1.84678) | 1 | 1 |
| G: -5311.84231 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.74382 HOMO: -6.68584 LUMO: 1.60275 factor:1 | 1 (-1.53581) | 1 | 1 |
| G: -5311.84231 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.70240 HOMO: -6.40556 LUMO: 1.45581 factor:1 | 1 (-1.49439) | -1 | -1 |
| G: -5311.84231 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11578.05517 HOMO: -6.94979 LUMO: 2.16603 factor:1 | 1 (-1.84716) | 1 | 1 |
| G: -5311.84231 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.78167 HOMO: -6.84911 LUMO: 1.89935 factor:1 | 1 (-1.57366) | 1 | 1 |
| G: -5311.84231 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.89421 HOMO: -6.22052 LUMO: 1.57282 factor:1 | 1 (-1.68621) | -1 | -1 |
| G: -5311.84231 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.70341 HOMO: -6.51168 LUMO: 2.10072 factor:1 | 1 (-1.49540) | -1 | -1 |
| G: -5311.84231 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.61546 HOMO: -7.03686 LUMO: 2.12249 factor:1 | 1 (-1.40745) | 1 | 1 |
| G: -5311.84231 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.47061 HOMO: -6.84094 LUMO: 1.63268 factor:1 | 1 (-1.26261) | 1 | 1 |
| G: -5311.84231 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.86670 HOMO: -6.75387 LUMO: 1.72248 factor:1 | 1 (-1.65870) | 1 | 1 |
| G: -5311.84231 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.66833 HOMO: -6.86271 LUMO: 1.68711 factor:1 | 1 (-1.46033) | 1 | 1 |
| G: -5311.84231 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.47921 HOMO: -6.84094 LUMO: 2.02997 factor:1 | 1 (-1.27121) | 1 | 1 |
| G: -5311.84231 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.68082 HOMO: -6.80557 LUMO: 2.02725 factor:1 | 1 (-1.47282) | 1 | 1 |
| G: -5311.84231 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.72773 HOMO: -6.38651 LUMO: 1.53472 factor:1 | 1 (-1.51973) | -1 | -1 |
| G: -5311.84231 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.64346 HOMO: -7.51306 LUMO: 0.28572 factor:1 | 1 (-1.43546) | -1 | -1 |
| G: -5311.84231 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.81846 HOMO: -6.97972 LUMO: -0.74287 factor:1 | 1 (-1.61045) | -1 | -1 |
| G: -5311.84231 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.85870 HOMO: -6.83822 LUMO: -0.65852 factor:1 | 1 (-1.65070) | -1 | -1 |
| G: -5311.84231 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.66534 HOMO: -6.71305 LUMO: -0.49525 factor:1 | 1 (-1.45733) | -1 | -1 |
| G: -5311.84231 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.54071 HOMO: -6.60692 LUMO: -0.22313 factor:1 | 1 (-1.33270) | -1 | -1 |
| G: -5311.84231 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.36441 HOMO: -7.20013 LUMO: 0.55239 factor:1 | 1 (-1.15640) | -1 | -1 |
| G: -5311.84231 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.77329 HOMO: -6.60420 LUMO: -0.28028 factor:1 | 1 (-1.56528) | -1 | -1 |
| G: -5311.84231 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.58389 HOMO: -6.69128 LUMO: -0.30477 factor:1 | 1 (-1.37589) | -1 | -1 |
| G: -5311.84231 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.74156 HOMO: -6.65591 LUMO: -0.25579 factor:1 | 1 (-1.53355) | -1 | -1 |
| G: -5311.84231 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.42620 HOMO: -6.69128 LUMO: 1.70888 factor:1 | 1 (-1.21820) | 1 | 1 |
| G: -5311.84231 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.33679 HOMO: -6.50080 LUMO: 1.87759 factor:1 | 1 (-1.12878) | -1 | -1 |
| G: -5311.84231 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.57853 HOMO: -6.85727 LUMO: 1.99187 factor:1 | 1 (-1.37053) | 1 | 1 |
| G: -5311.84231 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.45037 HOMO: -6.58788 LUMO: 1.79051 factor:1 | 1 (-1.24236) | 1 | 1 |
| G: -5311.84231 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.77092 HOMO: -6.64230 LUMO: 2.16058 factor:1 | 1 (-1.56291) | 1 | 1 |
| G: -5311.84231 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.41891 HOMO: -6.58788 LUMO: 2.10616 factor:1 | 1 (-1.21091) | 1 | 1 |
| G: -5311.84231 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.15923 HOMO: -7.01782 LUMO: 2.13609 factor:1 | 1 (-0.95123) | 1 | 1 |
| G: -5311.84231 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.44599 HOMO: -6.31304 LUMO: 2.31841 factor:1 | 1 (-1.23798) | -1 | -1 |
| G: -5311.84231 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.71337 HOMO: -6.94979 LUMO: 2.07895 factor:1 | 1 (-1.50536) | 1 | 1 |
| G: -5311.84231 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.48161 HOMO: -6.88992 LUMO: 2.28031 factor:1 | 1 (-1.27360) | 1 | 1 |
| G: -5311.84231 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.53709 HOMO: -6.66407 LUMO: 2.07623 factor:1 | 1 (-1.32909) | 1 | 1 |
| G: -5311.84231 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.56223 HOMO: -6.52529 LUMO: 1.70071 factor:1 | 1 (-1.35423) | -1 | -1 |
| G: -5311.84231 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.74335 HOMO: -6.58788 LUMO: 1.57282 factor:1 | 1 (-1.53535) | -1 | -1 |
| G: -5311.84231 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.69473 HOMO: -6.55250 LUMO: 1.95378 factor:1 | 1 (-1.48672) | -1 | -1 |
| G: -5311.84231 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.60112 HOMO: -6.24773 LUMO: 1.77962 factor:1 | 1 (-1.39311) | -1 | -1 |
| G: -5311.84231 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.88172 HOMO: -6.31304 LUMO: 2.18507 factor:1 | 1 (-1.67372) | -1 | -1 |
| G: -5311.84231 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.58727 HOMO: -6.18243 LUMO: 2.01636 factor:1 | 1 (-1.37926) | -1 | -1 |
| G: -5311.84231 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.75617 HOMO: -6.99877 LUMO: 2.14970 factor:1 | 1 (-1.54816) | 1 | 1 |
| G: -5311.84231 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.61453 HOMO: -6.72665 LUMO: 2.07079 factor:1 | 1 (-1.40653) | 1 | 1 |
| G: -5311.84231 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.53644 HOMO: -6.36202 LUMO: 2.17419 factor:1 | 1 (-1.32843) | -1 | -1 |
| G: -5311.84231 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.42729 HOMO: -6.78652 LUMO: 2.05718 factor:1 | 1 (-1.21929) | 1 | -1 |
| G: -5311.84231 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.44610 HOMO: -6.87360 LUMO: 2.34290 factor:1 | 1 (-1.23809) | 1 | 1 |
| G: -5311.84231 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.71035 HOMO: -6.62053 LUMO: 1.89391 factor:1 | 1 (-1.50234) | 1 | 1 |
| G: -5311.84231 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.81843 HOMO: -6.58788 LUMO: 1.83133 factor:1 | 1 (-1.61042) | 1 | 1 |
| G: -5311.84231 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.60485 HOMO: -7.08584 LUMO: 1.91568 factor:1 | 1 (-1.39684) | 1 | 1 |
| G: -5311.84231 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.39369 HOMO: -6.56883 LUMO: 1.81228 factor:1 | 1 (-1.18568) | 1 | 1 |
| G: -5311.84231 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.43410 HOMO: -6.66135 LUMO: 1.92384 factor:1 | 1 (-1.22609) | 1 | 1 |
| G: -5311.84231 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.32702 HOMO: -6.64502 LUMO: 2.15786 factor:1 | 1 (-1.11901) | 1 | 1 |
| G: -5311.84231 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.18974 HOMO: -6.71305 LUMO: 1.91840 factor:1 | 1 (-0.98173) | 1 | 1 |
| G: -5311.84231 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.70643 HOMO: -6.44094 LUMO: 1.74425 factor:1 | 1 (-1.49842) | -1 | -1 |
| G: -5311.84231 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.48514 HOMO: -6.51985 LUMO: 1.84221 factor:1 | 1 (-1.27714) | -1 | -1 |
| G: -5311.84231 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.14612 HOMO: -6.63414 LUMO: -0.24762 factor:1 | 1 (-0.93811) | -1 | -1 |
| G: -5311.84231 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.21548 HOMO: -6.60420 LUMO: -0.22585 factor:1 | 1 (-1.00747) | -1 | -1 |
| G: -5311.84231 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.52841 HOMO: -7.19741 LUMO: 0.58232 factor:1 | 1 (-1.32041) | -1 | -1 |
| G: -5311.84231 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.30457 HOMO: -6.77019 LUMO: -0.56872 factor:1 | 1 (-1.09656) | -1 | -1 |
| G: -5311.84231 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.37135 HOMO: -7.46136 LUMO: 0.28844 factor:1 | 1 (-1.16334) | -1 | -1 |
| G: -5311.84231 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11578.10940 HOMO: -6.60420 LUMO: -0.54151 factor:1 | 1 (-1.90140) | -1 | -1 |
| G: -5311.84231 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11578.39055 HOMO: -6.53890 LUMO: -0.46531 factor:1 | 1 (-2.18254) | -1 | -1 |
| G: -5311.84231 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11578.98925 HOMO: -6.81645 LUMO: -0.57144 factor:1 | 1 (-2.78125) | -1 | -1 |
| G: -5311.84231 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.70591 HOMO: -7.48041 LUMO: 0.28572 factor:1 | 1 (-1.49791) | -1 | -1 |
| G: -5311.84231 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11578.13473 HOMO: -6.75659 LUMO: -0.45715 factor:1 | 1 (-1.92673) | -1 | -1 |
| G: -5311.84231 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.74743 HOMO: -6.66135 LUMO: -0.41906 factor:1 | 1 (-1.53943) | -1 | -1 |
| G: -5311.84231 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11578.17299 HOMO: -6.55794 LUMO: -0.27483 factor:1 | 1 (-1.96499) | -1 | -1 |
| G: -5311.84231 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.99476 HOMO: -7.07496 LUMO: -0.63403 factor:1 | 1 (-1.78675) | -1 | -1 |
| G: -5311.84231 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11578.38946 HOMO: -7.12394 LUMO: 0.53334 factor:1 | 1 (-2.18146) | -1 | -1 |
| G: -5311.84231 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11578.93761 HOMO: -6.53617 LUMO: -0.25579 factor:1 | 1 (-2.72960) | -1 | -1 |
| G: -5311.84231 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11578.19879 HOMO: -6.50896 LUMO: -0.25034 factor:1 | 1 (-1.99079) | -1 | -1 |
| G: -5311.84231 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11578.45123 HOMO: -7.17564 LUMO: -0.68573 factor:1 | 1 (-2.24323) | -1 | -1 |
| G: -5311.84231 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11579.10898 HOMO: -6.53617 LUMO: -0.30749 factor:1 | 1 (-2.90098) | -1 | -1 |
| G: -5311.84231 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11578.98863 HOMO: -6.55522 LUMO: -0.30749 factor:1 | 1 (-2.78062) | -1 | -1 |
| G: -5311.84231 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.81339 HOMO: -7.05591 LUMO: -0.71022 factor:1 | 1 (-1.60539) | -1 | -1 |
| G: -5311.84231 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.96306 HOMO: -7.17564 LUMO: -0.69933 factor:1 | 1 (-1.75505) | -1 | -1 |
| G: -5311.84231 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11578.29947 HOMO: -6.78380 LUMO: -0.67756 factor:1 | 1 (-2.09147) | -1 | -1 |
| G: -5311.84231 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11578.18761 HOMO: -6.62325 LUMO: 2.02725 factor:1 | 1 (-1.97960) | 1 | 1 |
| G: -5311.84231 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.91223 HOMO: -6.63414 LUMO: 1.91296 factor:1 | 1 (-1.70422) | 1 | -1 |
| G: -5311.84231 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.69005 HOMO: -6.83278 LUMO: 1.65717 factor:1 | 1 (-0.48205) | 1 | 1 |
| G: -5311.84231 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.85564 HOMO: -6.66407 LUMO: 1.95650 factor:1 | 1 (-0.64763) | 1 | 1 |
| G: -5311.84231 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.10307 HOMO: -6.61237 LUMO: 2.11432 factor:1 | 1 (-0.89506) | 1 | 1 |
| G: -5311.84231 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.79169 HOMO: -6.62053 LUMO: 2.09256 factor:1 | 1 (-0.58368) | 1 | -1 |
| G: -5311.84231 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.60589 HOMO: -6.78652 LUMO: 2.13609 factor:1 | 1 (-0.39788) | 1 | 1 |
| G: -5311.84231 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.64028 HOMO: -6.94707 LUMO: 1.81772 factor:1 | 1 (-0.43228) | 1 | 1 |
| G: -5311.84231 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.65004 HOMO: -6.85183 LUMO: 2.12793 factor:1 | 1 (-1.44204) | 1 | 1 |
| G: -5311.84231 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11578.51580 HOMO: -6.81101 LUMO: 1.83949 factor:1 | 1 (-2.30780) | 1 | 1 |
| G: -5311.84231 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.97723 HOMO: -6.98788 LUMO: 2.16058 factor:1 | 1 (-1.76923) | 1 | 1 |
| G: -5311.84231 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.83108 HOMO: -6.62869 LUMO: 2.00820 factor:1 | 1 (-1.62308) | 1 | 1 |
| G: -5311.84231 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.58085 HOMO: -6.34025 LUMO: 2.25855 factor:1 | 1 (-1.37284) | -1 | -1 |
| G: -5311.84231 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.70308 HOMO: -6.01372 LUMO: 2.01636 factor:1 | 1 (-1.49508) | -1 | -1 |
| G: -5311.84231 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.59279 HOMO: -6.89264 LUMO: 2.27487 factor:1 | 1 (-1.38479) | 1 | 1 |
| G: -5311.84231 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.80050 HOMO: -6.53073 LUMO: 2.20684 factor:1 | 1 (-1.59249) | -1 | -1 |
| G: -5311.84231 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.65772 HOMO: -6.83278 LUMO: 1.53744 factor:1 | 1 (-1.44971) | -1 | -1 |
| G: -5311.84231 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.96877 HOMO: -6.41917 LUMO: 1.82316 factor:1 | 1 (-1.76077) | -1 | -1 |
| G: -5311.84231 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.76395 HOMO: -6.56339 LUMO: 1.63813 factor:1 | 1 (-1.55595) | -1 | -1 |
| G: -5311.84231 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11578.12815 HOMO: -6.88992 LUMO: 1.65173 factor:1 | 1 (-1.92014) | 1 | 1 |
| G: -5311.84231 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.97669 HOMO: -6.63141 LUMO: 1.92112 factor:1 | 1 (-1.76869) | 1 | 1 |
| G: -5311.84231 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11578.22407 HOMO: -6.83822 LUMO: 1.88847 factor:1 | 1 (-2.01606) | 1 | 1 |
| G: -5311.84231 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11578.80087 HOMO: -6.84638 LUMO: 1.90480 factor:1 | 1 (-2.59286) | 1 | 1 |
| G: -5311.84231 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11578.38970 HOMO: -6.82462 LUMO: 1.70888 factor:1 | 1 (-2.18170) | 1 | 1 |
| G: -5311.84231 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11578.15218 HOMO: -6.82734 LUMO: 2.12521 factor:1 | 1 (-1.94417) | 1 | 1 |
| G: -5311.84231 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.71168 HOMO: -6.94435 LUMO: 1.87214 factor:1 | 1 (-1.50367) | 1 | 1 |
| G: -5311.84231 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.95879 HOMO: -6.98516 LUMO: 2.51433 factor:1 | 1 (-1.75078) | 1 | 1 |
| G: -5311.84231 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.95217 HOMO: -6.74026 LUMO: 2.15514 factor:1 | 1 (-1.74417) | 1 | 1 |
| G: -5311.84231 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.82006 HOMO: -6.93618 LUMO: 2.54426 factor:1 | 1 (-1.61206) | 1 | 1 |
| G: -5311.84231 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.56789 HOMO: -6.28583 LUMO: 2.53610 factor:1 | 1 (-1.35989) | -1 | -1 |
| G: -5311.84231 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.91496 HOMO: -6.56883 LUMO: 1.94834 factor:1 | 1 (-0.70695) | 1 | 1 |
| G: -5311.84231 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.82407 HOMO: -7.08584 LUMO: 1.99187 factor:1 | 1 (-0.61607) | 1 | 1 |
| G: -5311.84231 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.93324 HOMO: -6.19059 LUMO: 1.99732 factor:1 | 1 (-0.72524) | -1 | -1 |
| G: -5311.84231 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.17480 HOMO: -6.78108 LUMO: 2.03813 factor:1 | 1 (-0.96679) | 1 | 1 |
| G: -5311.84231 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.12565 HOMO: -6.82189 LUMO: 1.77418 factor:1 | 1 (-0.91765) | 1 | 1 |
| G: -5311.84231 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.96225 HOMO: -6.45454 LUMO: 1.78779 factor:1 | 1 (-0.75425) | -1 | -1 |
| G: -5311.84231 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.93771 HOMO: -6.84366 LUMO: 1.77690 factor:1 | 1 (-0.72970) | 1 | 1 |
| G: -5311.84231 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.74475 HOMO: -6.74026 LUMO: 1.67622 factor:1 | 1 (-0.53674) | 1 | 1 |
| G: -5311.84231 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.76276 HOMO: -6.76475 LUMO: 2.40277 factor:1 | 1 (-0.55476) | 1 | 1 |
| G: -5311.84231 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.68878 HOMO: -6.65863 LUMO: 1.86670 factor:1 | 1 (-0.48077) | 1 | 1 |
| G: -5311.84231 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.82366 HOMO: -6.50080 LUMO: 1.93201 factor:1 | 1 (-0.61566) | -1 | -1 |
| G: -5311.84231 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.95049 HOMO: -6.34842 LUMO: 1.70888 factor:1 | 1 (-0.74249) | -1 | -1 |
| G: -5311.84231 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.92440 HOMO: -6.60692 LUMO: 2.20140 factor:1 | 1 (-0.71639) | 1 | 1 |
| G: -5311.84231 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.05412 HOMO: -6.74026 LUMO: 2.14970 factor:1 | 1 (-0.84611) | 1 | 1 |
| G: -5311.84231 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.09031 HOMO: -6.63686 LUMO: 2.17419 factor:1 | 1 (-0.88230) | 1 | 1 |
| G: -5311.84231 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.87694 HOMO: -6.81917 LUMO: 2.10072 factor:1 | 1 (-0.66894) | 1 | -1 |
| G: -5311.84231 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.82834 HOMO: -6.92802 LUMO: 2.04358 factor:1 | 1 (-0.62034) | 1 | 1 |
| G: -5311.84231 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.66026 HOMO: -6.56067 LUMO: -0.47620 factor:1 | 1 (-0.45225) | -1 | -1 |
| G: -5311.84231 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.80815 HOMO: -6.56611 LUMO: -0.77008 factor:1 | 1 (-0.60015) | -1 | -1 |
| G: -5311.84231 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.68761 HOMO: -6.78380 LUMO: -0.64763 factor:1 | 1 (-0.47960) | -1 | -1 |
| G: -5311.84231 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.85621 HOMO: -6.51985 LUMO: -0.24490 factor:1 | 1 (-0.64820) | -1 | -1 |
| G: -5311.84231 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.69539 HOMO: -6.52529 LUMO: -0.27483 factor:1 | 1 (-0.48738) | -1 | -1 |
| G: -5311.84231 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.11999 HOMO: -7.10489 LUMO: -0.62586 factor:1 | 1 (-0.91199) | -1 | -1 |
| G: -5311.84231 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.89506 HOMO: -7.18108 LUMO: 0.48980 factor:1 | 1 (-0.68706) | -1 | -1 |
| G: -5311.84231 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.90440 HOMO: -7.14299 LUMO: -0.63947 factor:1 | 1 (-0.69639) | -1 | -1 |
| G: -5311.84231 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.75476 HOMO: -6.70761 LUMO: -0.54423 factor:1 | 1 (-0.54676) | -1 | -1 |
| G: -5311.84231 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.67280 HOMO: -7.32258 LUMO: -1.03675 factor:1 | 1 (-0.46480) | -1 | -1 |
| G: -5311.84231 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.55190 HOMO: -6.65046 LUMO: -0.41361 factor:1 | 1 (-0.34390) | -1 | -1 |
| G: -5311.84231 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.70110 HOMO: -6.76475 LUMO: -0.60137 factor:1 | 1 (-0.49310) | -1 | -1 |
| G: -5311.84231 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.94277 HOMO: -6.77836 LUMO: -0.54423 factor:1 | 1 (-0.73476) | -1 | -1 |
| G: -5311.84231 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11578.14483 HOMO: -7.52395 LUMO: 0.26395 factor:1 | 1 (-1.93682) | -1 | -1 |
| G: -5311.84231 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11579.07984 HOMO: -6.93890 LUMO: -0.72382 factor:1 | 1 (-2.87184) | -1 | -1 |
| G: -5311.84231 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11578.29335 HOMO: -6.72938 LUMO: -0.47348 factor:1 | 1 (-2.08534) | -1 | -1 |
| G: -5311.84231 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11578.20937 HOMO: -6.66951 LUMO: -0.40817 factor:1 | 1 (-2.00137) | -1 | -1 |
| G: -5311.84231 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.98635 HOMO: -6.60420 LUMO: -0.19320 factor:1 | 1 (-1.77835) | -1 | -1 |
| G: -5311.84231 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.75493 HOMO: -6.67495 LUMO: -0.27211 factor:1 | 1 (-0.54692) | -1 | -1 |
| G: -5311.84231 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.73351 HOMO: -7.23823 LUMO: -0.62858 factor:1 | 1 (-0.52551) | -1 | -1 |
| G: -5311.84231 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.96571 HOMO: -7.27088 LUMO: 0.53334 factor:1 | 1 (-0.75770) | -1 | -1 |
| G: -5311.84231 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.84187 HOMO: -7.20013 LUMO: 0.59049 factor:1 | 1 (-0.63386) | -1 | -1 |
| G: -5311.84231 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.59903 HOMO: -6.60148 LUMO: -0.20953 factor:1 | 1 (-0.39103) | -1 | -1 |
| G: -5311.84231 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.50972 HOMO: -6.69400 LUMO: -0.51974 factor:1 | 1 (-0.30172) | -1 | -1 |
| G: -5311.84231 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.69416 HOMO: -7.40422 LUMO: -0.98777 factor:1 | 1 (-0.48616) | -1 | -1 |
| G: -5311.84231 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.87185 HOMO: -6.88176 LUMO: -0.71022 factor:1 | 1 (-0.66385) | -1 | -1 |
| G: -5311.84231 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.73758 HOMO: -6.86271 LUMO: -0.59321 factor:1 | 1 (-1.52958) | -1 | -1 |
| G: -5311.84231 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11578.44568 HOMO: -6.73754 LUMO: -0.55239 factor:1 | 1 (-2.23767) | -1 | -1 |
| G: -5311.84231 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.76953 HOMO: -6.71033 LUMO: 1.57010 factor:1 | 1 (-1.56153) | -1 | -1 |
| G: -5311.84231 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.97966 HOMO: -6.69672 LUMO: 1.68711 factor:1 | 1 (-1.77165) | 1 | 1 |
| G: -5311.84231 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.87266 HOMO: -6.67495 LUMO: 2.03813 factor:1 | 1 (-1.66466) | 1 | 1 |
| G: -5311.84231 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.59456 HOMO: -6.54434 LUMO: 1.83677 factor:1 | 1 (-1.38656) | -1 | -1 |
| G: -5311.84231 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.75707 HOMO: -6.57155 LUMO: 1.77146 factor:1 | 1 (-1.54906) | 1 | 1 |
| G: -5311.84231 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.92602 HOMO: -6.76747 LUMO: 1.87759 factor:1 | 1 (-1.71802) | 1 | 1 |
| G: -5311.84231 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.78575 HOMO: -6.58243 LUMO: 1.61364 factor:1 | 1 (-1.57774) | 1 | 1 |
| G: -5311.84231 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.54844 HOMO: -6.61781 LUMO: 2.13881 factor:1 | 1 (-1.34043) | 1 | 1 |
| G: -5311.84231 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11578.10545 HOMO: -6.62597 LUMO: 2.00276 factor:1 | 1 (-1.89745) | 1 | 1 |
| G: -5311.84231 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.93704 HOMO: -7.01237 LUMO: 1.95922 factor:1 | 1 (-1.72904) | 1 | 1 |
| G: -5311.84231 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11578.16984 HOMO: -7.03959 LUMO: 2.16875 factor:1 | 1 (-1.96183) | 1 | 1 |
| G: -5311.84231 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.91927 HOMO: -6.83278 LUMO: 1.91296 factor:1 | 1 (-1.71127) | 1 | 1 |
| G: -5311.84231 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11578.07949 HOMO: -6.40012 LUMO: 1.95650 factor:1 | 1 (-1.87149) | -1 | -1 |
| G: -5311.84231 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.76567 HOMO: -6.50080 LUMO: 1.73337 factor:1 | 1 (-0.55767) | -1 | -1 |
| G: -5311.84231 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.54853 HOMO: -6.95795 LUMO: 2.28848 factor:1 | 1 (-0.34052) | 1 | 1 |
| G: -5311.84231 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.85596 HOMO: -6.63686 LUMO: 2.20140 factor:1 | 1 (-0.64796) | 1 | -1 |
| G: -5311.84231 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.59808 HOMO: -6.57427 LUMO: 1.87214 factor:1 | 1 (-0.39008) | 1 | -1 |
| G: -5311.84231 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.81115 HOMO: -6.38379 LUMO: 2.32113 factor:1 | 1 (-0.60314) | -1 | -1 |
| G: -5311.84231 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.78461 HOMO: -6.63958 LUMO: 2.04902 factor:1 | 1 (-0.57661) | 1 | 1 |
| G: -5311.84231 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.56692 HOMO: -6.70216 LUMO: 1.93201 factor:1 | 1 (-0.35892) | 1 | 1 |
| G: -5311.84231 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.54436 HOMO: -6.80557 LUMO: 2.23678 factor:1 | 1 (-0.33636) | 1 | 1 |
| G: -5311.84231 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.34899 HOMO: -6.72938 LUMO: 2.28304 factor:1 | 1 (-0.14098) | 1 | 1 |
| G: -5311.84231 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.72344 HOMO: -6.56067 LUMO: 1.66806 factor:1 | 1 (-0.51544) | -1 | -1 |
| G: -5311.84231 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.74235 HOMO: -6.95523 LUMO: 2.33474 factor:1 | 1 (-1.53434) | 1 | 1 |
| G: -5311.84231 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.55516 HOMO: -6.59876 LUMO: 2.30480 factor:1 | 1 (-1.34715) | 1 | 1 |
| G: -5311.84231 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11578.59292 HOMO: -6.87360 LUMO: 1.75786 factor:1 | 1 (-2.38491) | 1 | 1 |
| G: -5311.84231 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.58553 HOMO: -7.06408 LUMO: 1.99187 factor:1 | 1 (-1.37752) | 1 | 1 |
| G: -5311.84231 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.82621 HOMO: -6.95795 LUMO: 1.88847 factor:1 | 1 (-1.61821) | 1 | 1 |
| G: -5311.84231 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.78539 HOMO: -6.85455 LUMO: 1.63813 factor:1 | 1 (-1.57739) | 1 | 1 |
| G: -5311.84231 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.81100 HOMO: -7.09129 LUMO: 2.31569 factor:1 | 1 (-1.60300) | 1 | 1 |
| G: -5311.84231 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.61336 HOMO: -6.91441 LUMO: 1.68983 factor:1 | 1 (-1.40536) | 1 | 1 |
| G: -5311.84231 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.80537 HOMO: -6.89809 LUMO: 2.23678 factor:1 | 1 (-1.59736) | 1 | 1 |
| G: -5311.84231 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.02780 HOMO: -6.78652 LUMO: 1.98371 factor:1 | 1 (-0.81980) | 1 | -1 |
| G: -5311.84231 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.89789 HOMO: -6.94707 LUMO: 2.23678 factor:1 | 1 (-0.68989) | 1 | 1 |
| G: -5311.84231 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.94946 HOMO: -7.07224 LUMO: 2.13337 factor:1 | 1 (-0.74146) | 1 | 1 |
| G: -5311.84231 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.06759 HOMO: -6.94979 LUMO: 2.28031 factor:1 | 1 (-0.85958) | 1 | 1 |
| G: -5311.84231 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.90641 HOMO: -6.60965 LUMO: 2.20412 factor:1 | 1 (-0.69841) | 1 | 1 |
| G: -5311.84231 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.71041 HOMO: -6.87360 LUMO: 2.40277 factor:1 | 1 (-0.50240) | 1 | -1 |
| G: -5311.84231 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.81270 HOMO: -6.92802 LUMO: 1.89663 factor:1 | 1 (-0.60469) | 1 | -1 |
| G: -5311.84231 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.96054 HOMO: -6.88448 LUMO: 2.02725 factor:1 | 1 (-0.75253) | 1 | 1 |
| G: -5311.84231 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.21268 HOMO: -6.69128 LUMO: 1.55105 factor:1 | 1 (-1.00467) | -1 | -1 |
| G: -5311.84231 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.08187 HOMO: -6.54978 LUMO: 1.93201 factor:1 | 1 (-0.87387) | -1 | -1 |
| G: -5311.84231 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.20574 HOMO: -6.19331 LUMO: 1.46941 factor:1 | 1 (-0.99773) | -1 | -1 |
| G: -5311.84231 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.07199 HOMO: -6.55794 LUMO: 1.89663 factor:1 | 1 (-0.86399) | -1 | -1 |
| G: -5311.84231 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.04816 HOMO: -6.07630 LUMO: 1.94289 factor:1 | 1 (-0.84015) | -1 | -1 |
| G: -5311.84231 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.85226 HOMO: -7.46408 LUMO: 0.31565 factor:1 | 1 (-0.64426) | -1 | -1 |
| G: -5311.84231 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.98435 HOMO: -6.63958 LUMO: -0.61770 factor:1 | 1 (-0.77634) | -1 | -1 |
| G: -5311.84231 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.01730 HOMO: -6.81101 LUMO: -0.57960 factor:1 | 1 (-0.80929) | -1 | -1 |
| G: -5311.84231 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.18955 HOMO: -6.74298 LUMO: -0.57960 factor:1 | 1 (-0.98154) | -1 | -1 |
| G: -5311.84231 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.97814 HOMO: -6.63686 LUMO: -0.42994 factor:1 | 1 (-0.77014) | -1 | -1 |
| G: -5311.84231 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.21940 HOMO: -6.60965 LUMO: -0.41089 factor:1 | 1 (-1.01139) | -1 | -1 |
| G: -5311.84231 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.05120 HOMO: -6.60692 LUMO: -0.80274 factor:1 | 1 (-0.84320) | -1 | -1 |
| G: -5311.84231 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.80480 HOMO: -6.58788 LUMO: -0.78097 factor:1 | 1 (-0.59680) | -1 | -1 |
| G: -5311.84231 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.98315 HOMO: -6.67767 LUMO: -0.48436 factor:1 | 1 (-0.77514) | -1 | -1 |
| G: -5311.84231 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.86979 HOMO: -6.63141 LUMO: -0.40545 factor:1 | 1 (-0.66178) | -1 | -1 |
| G: -5311.84231 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.76970 HOMO: -6.62053 LUMO: -0.83811 factor:1 | 1 (-0.56170) | -1 | -1 |
| G: -5311.84231 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.98927 HOMO: -6.59604 LUMO: -0.35375 factor:1 | 1 (-0.78127) | -1 | -1 |
| G: -5311.84231 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.84516 HOMO: -6.34297 LUMO: -0.39729 factor:1 | 1 (-0.63715) | -1 | -1 |
| G: -5311.84231 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.12816 HOMO: -6.67223 LUMO: 1.97827 factor:1 | 1 (-0.92015) | 1 | 1 |
| G: -5311.84231 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.92805 HOMO: -6.40012 LUMO: 1.89935 factor:1 | 1 (-0.72004) | -1 | -1 |
| G: -5311.84231 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.12729 HOMO: -6.74842 LUMO: 1.97283 factor:1 | 1 (-0.91928) | 1 | -1 |
| G: -5311.84231 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.93028 HOMO: -6.76747 LUMO: 2.17147 factor:1 | 1 (-0.72227) | 1 | 1 |
| G: -5311.84231 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.77710 HOMO: -6.72121 LUMO: 1.55649 factor:1 | 1 (-0.56910) | -1 | -1 |
| G: -5311.84231 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.84151 HOMO: -6.97700 LUMO: 2.04085 factor:1 | 1 (-0.63351) | 1 | 1 |
| G: -5311.84231 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.59060 HOMO: -7.06680 LUMO: 2.04085 factor:1 | 1 (-0.38259) | 1 | -1 |
| G: -5311.84231 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.63027 HOMO: -7.09673 LUMO: 2.35106 factor:1 | 1 (-0.42227) | 1 | 1 |
| G: -5311.84231 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.60276 HOMO: -6.83006 LUMO: 2.14970 factor:1 | 1 (-0.39476) | 1 | 1 |
| G: -5311.84231 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.47770 HOMO: -6.72665 LUMO: 2.20140 factor:1 | 1 (-0.26969) | 1 | -1 |
| G: -5311.84231 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.97346 HOMO: -6.77291 LUMO: 2.34562 factor:1 | 1 (-0.76546) | 1 | -1 |
| G: -5311.84231 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.07588 HOMO: -6.73754 LUMO: 2.00276 factor:1 | 1 (-0.86788) | 1 | -1 |
| G: -5311.84231 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.02892 HOMO: -7.04231 LUMO: 1.92112 factor:1 | 1 (-0.82091) | 1 | -1 |
| G: -5311.84231 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.90965 HOMO: -6.83822 LUMO: 1.72248 factor:1 | 1 (-0.70165) | 1 | 1 |
| G: -5311.84231 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.13540 HOMO: -6.57971 LUMO: 2.16603 factor:1 | 1 (-0.92739) | 1 | -1 |
| G: -5311.84231 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.24680 HOMO: -6.80013 LUMO: 1.88575 factor:1 | 1 (-1.03879) | 1 | 1 |
| G: -5311.84231 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.13428 HOMO: -6.93618 LUMO: 2.18235 factor:1 | 1 (-0.92628) | 1 | 1 |
| G: -5311.84231 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.15844 HOMO: -6.54706 LUMO: 1.91024 factor:1 | 1 (-0.95044) | -1 | -1 |
| G: -5311.84231 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.02046 HOMO: -7.06952 LUMO: 2.18507 factor:1 | 1 (-0.81245) | 1 | 1 |
| G: -5311.84231 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.83944 HOMO: -7.05047 LUMO: 1.82044 factor:1 | 1 (-0.63144) | 1 | 1 |
| G: -5311.84231 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.77604 HOMO: -6.87632 LUMO: 1.92657 factor:1 | 1 (-0.56804) | 1 | 1 |
| G: -5311.84231 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.79210 HOMO: -6.58788 LUMO: 1.91568 factor:1 | 1 (-0.58409) | 1 | -1 |
| G: -5311.84231 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.98617 HOMO: -7.17292 LUMO: 1.90752 factor:1 | 1 (-0.77816) | 1 | 1 |
| G: -5311.84231 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.66085 HOMO: -6.93890 LUMO: 1.80684 factor:1 | 1 (-1.45284) | 1 | 1 |
| G: -5311.84231 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.42819 HOMO: -7.10761 LUMO: 2.20956 factor:1 | 1 (-1.22019) | 1 | 1 |
| G: -5311.84231 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.75987 HOMO: -6.85727 LUMO: 2.13609 factor:1 | 1 (-1.55187) | 1 | -1 |
| G: -5311.84231 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.91451 HOMO: -6.64502 LUMO: 1.38506 factor:1 | 1 (-1.70651) | -1 | -1 |
| G: -5311.84231 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.72196 HOMO: -6.87360 LUMO: 1.15648 factor:1 | 1 (-1.51396) | -1 | -1 |
| G: -5311.84231 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.96485 HOMO: -6.67223 LUMO: 2.07351 factor:1 | 1 (-1.75685) | 1 | 1 |
| G: -5311.84231 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.49037 HOMO: -6.29671 LUMO: 2.43270 factor:1 | 1 (-1.28236) | -1 | -1 |
| G: -5311.84231 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.46819 HOMO: -6.90897 LUMO: 2.28848 factor:1 | 1 (-1.26019) | 1 | 1 |
| G: -5311.84231 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.34155 HOMO: -7.04231 LUMO: 1.70071 factor:1 | 1 (-1.13354) | 1 | 1 |
| G: -5311.84231 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.64501 HOMO: -6.69944 LUMO: 1.94834 factor:1 | 1 (-1.43701) | 1 | 1 |
| G: -5311.84231 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.70632 HOMO: -6.56067 LUMO: 2.20956 factor:1 | 1 (-1.49831) | -1 | -1 |
| G: -5311.84231 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.79822 HOMO: -6.65046 LUMO: 2.06807 factor:1 | 1 (-0.59021) | 1 | -1 |
| G: -5311.84231 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.84396 HOMO: -7.08584 LUMO: 1.98915 factor:1 | 1 (-0.63596) | 1 | 1 |
| G: -5311.84231 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.08105 HOMO: -6.69400 LUMO: 2.09256 factor:1 | 1 (-0.87305) | 1 | 1 |
| G: -5311.84231 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.68439 HOMO: -6.62869 LUMO: 2.16331 factor:1 | 1 (-0.47639) | 1 | 1 |
| G: -5311.84231 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.87164 HOMO: -6.85183 LUMO: 2.16058 factor:1 | 1 (-0.66363) | 1 | 1 |
| G: -5311.84231 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.73591 HOMO: -6.54706 LUMO: 1.92384 factor:1 | 1 (-0.52790) | -1 | -1 |
| G: -5311.84231 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.89139 HOMO: -6.84366 LUMO: 2.48984 factor:1 | 1 (-0.68339) | 1 | 1 |
| G: -5311.84231 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.15583 HOMO: -6.77291 LUMO: 2.46263 factor:1 | 1 (-0.94783) | 1 | 1 |
| G: -5311.84231 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.85346 HOMO: -7.01782 LUMO: 2.31025 factor:1 | 1 (-0.64545) | 1 | 1 |
| G: -5311.84231 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.84862 HOMO: -6.94707 LUMO: 2.29664 factor:1 | 1 (-0.64061) | 1 | 1 |
| G: -5311.84231 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.71857 HOMO: -6.64230 LUMO: 1.97283 factor:1 | 1 (-0.51057) | 1 | 1 |
| G: -5311.84231 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.41503 HOMO: -6.47359 LUMO: 2.20412 factor:1 | 1 (-0.20702) | -1 | -1 |
| G: -5311.84231 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.74089 HOMO: -6.90625 LUMO: 1.92384 factor:1 | 1 (-0.53288) | 1 | 1 |
| G: -5311.84231 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.96562 HOMO: -7.17020 LUMO: 2.06807 factor:1 | 1 (-0.75762) | 1 | 1 |
| G: -5311.84231 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.63555 HOMO: -6.65046 LUMO: 2.20956 factor:1 | 1 (-0.42755) | 1 | -1 |
| G: -5311.84231 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.75743 HOMO: -7.07496 LUMO: 1.82861 factor:1 | 1 (-0.54943) | 1 | 1 |
| G: -5311.84231 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.54842 HOMO: -6.83006 LUMO: 2.14970 factor:1 | 1 (-0.34041) | 1 | -1 |
| G: -5311.84231 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.11017 HOMO: -6.92802 LUMO: 1.99187 factor:1 | 1 (-0.90217) | 1 | 1 |
| G: -5311.84231 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.75640 HOMO: -6.69672 LUMO: 2.36739 factor:1 | 1 (-0.54839) | 1 | -1 |
| G: -5311.84231 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.62377 HOMO: -7.13755 LUMO: 2.00276 factor:1 | 1 (-0.41576) | 1 | 1 |
| G: -5311.84231 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.77509 HOMO: -6.92530 LUMO: 2.25582 factor:1 | 1 (-0.56709) | 1 | 1 |
| G: -5311.84231 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.97354 HOMO: -6.77564 LUMO: 1.97827 factor:1 | 1 (-0.76554) | 1 | 1 |
| G: -5311.84231 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.72023 HOMO: -6.87904 LUMO: 1.60003 factor:1 | 1 (-0.51223) | 1 | 1 |
| G: -5311.84231 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.50423 HOMO: -6.62869 LUMO: 1.90480 factor:1 | 1 (-0.29622) | 1 | 1 |
| G: -5311.84231 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.76668 HOMO: -6.71033 LUMO: 1.54833 factor:1 | 1 (-0.55868) | -1 | -1 |
| G: -5311.84231 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.78328 HOMO: -6.74298 LUMO: 1.47486 factor:1 | 1 (-0.57528) | -1 | -1 |
| G: -5311.84231 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.83596 HOMO: -6.77019 LUMO: 1.90480 factor:1 | 1 (-0.62796) | 1 | 1 |
| G: -5311.84231 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.87879 HOMO: -6.70489 LUMO: 1.99459 factor:1 | 1 (-0.67079) | 1 | 1 |
| G: -5311.84231 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.06726 HOMO: -6.73482 LUMO: 2.08711 factor:1 | 1 (-0.85925) | 1 | 1 |
| G: -5311.84231 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.90992 HOMO: -6.46543 LUMO: 1.73881 factor:1 | 1 (-0.70192) | -1 | -1 |
| G: -5311.84231 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.82649 HOMO: -6.96067 LUMO: 2.26127 factor:1 | 1 (-0.61849) | 1 | 1 |
| G: -5311.84231 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.70554 HOMO: -6.67767 LUMO: 2.10616 factor:1 | 1 (-0.49753) | 1 | 1 |
| G: -5311.84231 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.90200 HOMO: -6.28855 LUMO: 2.35923 factor:1 | 1 (-0.69400) | -1 | -1 |
| G: -5311.84231 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.74407 HOMO: -6.80285 LUMO: 1.62724 factor:1 | 1 (-0.53606) | 1 | 1 |
| G: -5311.84231 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.78516 HOMO: -6.85455 LUMO: 2.23133 factor:1 | 1 (-0.57715) | 1 | 1 |
| G: -5311.84231 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.54807 HOMO: -6.51713 LUMO: 2.33474 factor:1 | 1 (-0.34006) | -1 | -1 |
| G: -5311.84231 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.60782 HOMO: -6.88176 LUMO: 2.15242 factor:1 | 1 (-0.39982) | 1 | 1 |
| G: -5311.84231 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.43008 HOMO: -6.54434 LUMO: 2.32113 factor:1 | 1 (-0.22207) | -1 | -1 |
| G: -5311.84231 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.74780 HOMO: -6.62597 LUMO: 2.24222 factor:1 | 1 (-0.53979) | 1 | 1 |
| G: -5311.84231 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.09861 HOMO: -6.74570 LUMO: 2.19868 factor:1 | 1 (-0.89060) | 1 | 1 |
| G: -5311.84231 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.96581 HOMO: -6.62869 LUMO: 1.98915 factor:1 | 1 (-0.75781) | 1 | 1 |
| G: -5311.84231 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.06669 HOMO: -6.64502 LUMO: 2.13881 factor:1 | 1 (-0.85868) | 1 | 1 |
| G: -5311.84231 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.95052 HOMO: -6.95795 LUMO: 1.82316 factor:1 | 1 (-0.74252) | 1 | 1 |
| G: -5311.84231 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.89381 HOMO: -6.77291 LUMO: 1.36329 factor:1 | 1 (-0.68581) | -1 | -1 |
| G: -5311.84231 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.75468 HOMO: -6.45726 LUMO: 1.73064 factor:1 | 1 (-0.54668) | -1 | -1 |
| G: -5311.84231 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.78323 HOMO: -6.49264 LUMO: 1.77418 factor:1 | 1 (-0.57522) | -1 | -1 |
| G: -5311.84231 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.71925 HOMO: -6.60420 LUMO: 2.20956 factor:1 | 1 (-0.51125) | 1 | 1 |
| G: -5311.84231 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.99975 HOMO: -6.56067 LUMO: 2.05718 factor:1 | 1 (-0.79174) | -1 | -1 |
| G: -5311.84231 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.68366 HOMO: -6.62597 LUMO: 1.70343 factor:1 | 1 (-0.47566) | 1 | 1 |
| G: -5311.84231 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.91482 HOMO: -6.69400 LUMO: 2.16875 factor:1 | 1 (-0.70682) | 1 | 1 |
| G: -5311.84231 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.63188 HOMO: -6.63958 LUMO: 2.11977 factor:1 | 1 (-0.42387) | 1 | 1 |
| G: -5311.84231 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.78793 HOMO: -6.92802 LUMO: 1.82044 factor:1 | 1 (-0.57993) | 1 | -1 |
| G: -5311.84231 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.48265 HOMO: -6.56339 LUMO: 2.30480 factor:1 | 1 (-0.27464) | -1 | -1 |
| G: -5311.84231 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.77427 HOMO: -6.63958 LUMO: 1.91024 factor:1 | 1 (-0.56627) | 1 | -1 |
| G: -5311.84231 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.60766 HOMO: -6.93074 LUMO: 2.05446 factor:1 | 1 (-0.39965) | 1 | 1 |
| G: -5311.84231 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.65694 HOMO: -6.61509 LUMO: 2.03813 factor:1 | 1 (-0.44893) | 1 | 1 |
| G: -5311.84231 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.39843 HOMO: -6.61237 LUMO: 1.91296 factor:1 | 1 (-0.19043) | 1 | -1 |
| G: -5311.84231 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.97479 HOMO: -6.86815 LUMO: 1.95378 factor:1 | 1 (-0.76679) | 1 | 1 |
| G: -5311.84231 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.03743 HOMO: -6.63686 LUMO: 1.70888 factor:1 | 1 (-0.82943) | 1 | 1 |
| G: -5311.84231 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.13760 HOMO: -6.57971 LUMO: 2.20140 factor:1 | 1 (-0.92960) | 1 | -1 |
| G: -5311.84231 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.09050 HOMO: -6.41100 LUMO: 1.96738 factor:1 | 1 (-0.88249) | -1 | -1 |
| G: -5311.84231 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.11341 HOMO: -6.90081 LUMO: 1.65989 factor:1 | 1 (-0.90540) | 1 | 1 |
| G: -5311.84231 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.85264 HOMO: -6.68312 LUMO: 1.97827 factor:1 | 1 (-0.64464) | 1 | -1 |
| G: -5311.84231 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.86195 HOMO: -6.65318 LUMO: 2.10888 factor:1 | 1 (-0.65394) | 1 | -1 |
| G: -5311.84231 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.26843 HOMO: -6.62053 LUMO: 2.28848 factor:1 | 1 (-1.06043) | 1 | -1 |
| G: -5311.84231 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.09311 HOMO: -6.65863 LUMO: 2.29664 factor:1 | 1 (-0.88510) | 1 | -1 |
| G: -5311.84231 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.16642 HOMO: -6.63958 LUMO: 2.07623 factor:1 | 1 (-0.95841) | 1 | -1 |
| G: -5311.84231 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.03765 HOMO: -6.58243 LUMO: 2.20684 factor:1 | 1 (-0.82965) | 1 | 1 |
| G: -5311.84231 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.96701 HOMO: -6.59332 LUMO: 2.05174 factor:1 | 1 (-0.75901) | 1 | -1 |
| G: -5311.84231 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.95469 HOMO: -6.95251 LUMO: 2.20140 factor:1 | 1 (-0.74668) | 1 | 1 |
| G: -5311.84231 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.96048 HOMO: -6.84638 LUMO: 2.39732 factor:1 | 1 (-0.75248) | 1 | 1 |
| G: -5311.84231 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.07602 HOMO: -6.86815 LUMO: 2.47896 factor:1 | 1 (-0.86802) | 1 | 1 |
| G: -5311.84231 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.20103 HOMO: -7.00693 LUMO: 2.43270 factor:1 | 1 (-0.99303) | 1 | 1 |
| G: -5311.84231 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.24808 HOMO: -6.58788 LUMO: 2.30208 factor:1 | 1 (-1.04007) | 1 | 1 |
| G: -5311.84231 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.09031 HOMO: -6.63958 LUMO: 2.28031 factor:1 | 1 (-0.88230) | 1 | 1 |
| G: -5311.84231 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.04266 HOMO: -6.74570 LUMO: 2.28304 factor:1 | 1 (-0.83465) | 1 | 1 |
| G: -5311.84231 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.75539 HOMO: -6.78380 LUMO: 2.16331 factor:1 | 1 (-0.54738) | 1 | 1 |
| G: -5311.84231 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.75144 HOMO: -6.52529 LUMO: 2.05718 factor:1 | 1 (-0.54344) | -1 | -1 |
| G: -5311.84231 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.83623 HOMO: -6.41644 LUMO: 1.65445 factor:1 | 1 (-0.62823) | -1 | -1 |
| G: -5311.84231 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.10974 HOMO: -6.34570 LUMO: 1.22451 factor:1 | 1 (-0.90173) | -1 | -1 |
| G: -5311.84231 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.86965 HOMO: -6.14433 LUMO: 1.85582 factor:1 | 1 (-0.66164) | -1 | -1 |
| G: -5311.84231 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.16359 HOMO: -6.62053 LUMO: 1.92112 factor:1 | 1 (-0.95558) | 1 | -1 |
| G: -5311.84231 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.74208 HOMO: -6.63414 LUMO: 1.61908 factor:1 | 1 (-0.53408) | 1 | 1 |
| G: -5311.84231 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.93556 HOMO: -6.75931 LUMO: 1.87214 factor:1 | 1 (-0.72755) | 1 | 1 |
| G: -5311.84231 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.76067 HOMO: -6.55794 LUMO: 1.77418 factor:1 | 1 (-0.55266) | -1 | -1 |
| G: -5311.84231 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.54066 HOMO: -6.52801 LUMO: 1.82044 factor:1 | 1 (-0.33266) | -1 | -1 |
| G: -5311.84231 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.68371 HOMO: -6.77564 LUMO: 1.97827 factor:1 | 1 (-0.47571) | 1 | 1 |
| G: -5311.84231 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.86832 HOMO: -6.93890 LUMO: 1.81228 factor:1 | 1 (-0.66031) | 1 | 1 |
| G: -5311.84231 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.85022 HOMO: -6.85455 LUMO: 1.75513 factor:1 | 1 (-0.64222) | 1 | 1 |
| G: -5311.84231 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.12492 HOMO: -6.86815 LUMO: 1.64629 factor:1 | 1 (-0.91691) | 1 | 1 |
| G: -5311.84231 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.86192 HOMO: -6.98516 LUMO: 1.84765 factor:1 | 1 (-0.65392) | 1 | 1 |
| G: -5311.84231 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.96160 HOMO: -6.04637 LUMO: 1.94017 factor:1 | 1 (-0.75359) | -1 | -1 |
| G: -5311.84231 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.74148 HOMO: -6.86271 LUMO: 2.11977 factor:1 | 1 (-0.53348) | 1 | -1 |
| G: -5311.84231 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.05752 HOMO: -6.72938 LUMO: 2.11160 factor:1 | 1 (-0.84951) | 1 | -1 |
| G: -5311.84231 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.20187 HOMO: -7.01782 LUMO: 2.13609 factor:1 | 1 (-0.99387) | 1 | 1 |
| G: -5311.84231 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.82102 HOMO: -6.18515 LUMO: 2.04630 factor:1 | 1 (-0.61302) | -1 | -1 |
| G: -5311.84231 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.64412 HOMO: -6.60965 LUMO: 2.17147 factor:1 | 1 (-0.43612) | 1 | -1 |
| G: -5311.84231 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.94372 HOMO: -6.87360 LUMO: 2.35378 factor:1 | 1 (-0.73571) | 1 | 1 |
| G: -5311.84231 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.71166 HOMO: -6.72938 LUMO: 2.20140 factor:1 | 1 (-0.50366) | 1 | -1 |
| G: -5311.84231 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.63095 HOMO: -6.88448 LUMO: 2.54154 factor:1 | 1 (-0.42295) | 1 | -1 |
| G: -5311.84231 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.45688 HOMO: -6.87087 LUMO: 2.16058 factor:1 | 1 (-0.24888) | 1 | 1 |
| G: -5311.84231 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.96328 HOMO: -7.11306 LUMO: 2.04085 factor:1 | 1 (-0.75528) | 1 | 1 |
| G: -5311.84231 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.91428 HOMO: -6.66951 LUMO: 1.68438 factor:1 | 1 (-0.70627) | 1 | 1 |
| G: -5311.84231 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.16329 HOMO: -7.08312 LUMO: 2.19324 factor:1 | 1 (-0.95528) | 1 | 1 |
| G: -5311.84231 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.81452 HOMO: -6.69128 LUMO: 2.13881 factor:1 | 1 (-0.60651) | 1 | -1 |
| G: -5311.84231 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.68905 HOMO: -6.80285 LUMO: 2.16603 factor:1 | 1 (-0.48104) | 1 | 1 |
| G: -5311.84231 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.73563 HOMO: -6.82189 LUMO: 2.46807 factor:1 | 1 (-0.52763) | 1 | 1 |
| G: -5311.84231 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.96845 HOMO: -6.78652 LUMO: 2.12521 factor:1 | 1 (-0.76045) | 1 | 1 |
| G: -5311.84231 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.71142 HOMO: -6.47903 LUMO: 1.70071 factor:1 | 1 (-0.50341) | -1 | -1 |
| G: -5311.84231 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.72592 HOMO: -6.37019 LUMO: 1.24356 factor:1 | 1 (-0.51791) | -1 | -1 |
| G: -5311.84231 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.52129 HOMO: -6.69400 LUMO: 1.67350 factor:1 | 1 (-0.31328) | 1 | 1 |
| G: -5311.84231 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.59177 HOMO: -7.51851 LUMO: 0.27756 factor:1 | 1 (-0.38376) | -1 | -1 |
| G: -5311.84231 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.54140 HOMO: -6.95795 LUMO: -0.72110 factor:1 | 1 (-0.33339) | -1 | -1 |
| G: -5311.84231 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.32188 HOMO: -6.88720 LUMO: -0.67484 factor:1 | 1 (-0.11388) | -1 | -1 |
| G: -5311.84231 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.75631 HOMO: -6.83550 LUMO: -0.57144 factor:1 | 1 (-0.54831) | -1 | -1 |
| G: -5311.84231 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.63870 HOMO: -6.80285 LUMO: -0.57144 factor:1 | 1 (-1.43069) | -1 | -1 |
| G: -5311.84231 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.80153 HOMO: -6.76475 LUMO: -0.53062 factor:1 | 1 (-1.59353) | -1 | -1 |
| G: -5311.84231 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.67432 HOMO: -6.66951 LUMO: 1.74969 factor:1 | 1 (-1.46631) | 1 | 1 |
| G: -5311.84231 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.73644 HOMO: -6.53345 LUMO: 1.89935 factor:1 | 1 (-1.52844) | -1 | -1 |
| G: -5311.84231 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.96877 HOMO: -6.65046 LUMO: 2.01364 factor:1 | 1 (-1.76077) | 1 | -1 |
| G: -5311.84231 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.95876 HOMO: -6.64230 LUMO: 2.11977 factor:1 | 1 (-1.75075) | 1 | -1 |
| G: -5311.84231 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.90872 HOMO: -6.44910 LUMO: 2.13337 factor:1 | 1 (-1.70071) | -1 | -1 |
| G: -5311.84231 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.92774 HOMO: -7.05591 LUMO: 1.98915 factor:1 | 1 (-1.71973) | 1 | -1 |
| G: -5311.84231 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.65769 HOMO: -7.02326 LUMO: 2.49256 factor:1 | 1 (-1.44969) | 1 | 1 |
| G: -5311.84231 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.63043 HOMO: -6.32937 LUMO: 2.51161 factor:1 | 1 (-1.42242) | -1 | -1 |
| G: -5311.84231 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.45026 HOMO: -6.96067 LUMO: 2.20140 factor:1 | 1 (-1.24225) | 1 | 1 |
| G: -5311.84231 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.56498 HOMO: -6.97972 LUMO: 2.55243 factor:1 | 1 (-1.35698) | 1 | 1 |
| G: -5311.84231 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.49097 HOMO: -6.72665 LUMO: 2.46535 factor:1 | 1 (-1.28296) | 1 | 1 |
| G: -5311.84231 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.48065 HOMO: -6.41917 LUMO: 2.35106 factor:1 | 1 (-1.27265) | -1 | -1 |
| G: -5311.84231 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.65290 HOMO: -6.75114 LUMO: 2.32929 factor:1 | 1 (-1.44490) | 1 | 1 |
| G: -5311.84231 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.98152 HOMO: -6.91713 LUMO: 2.27215 factor:1 | 1 (-0.77351) | 1 | 1 |
| G: -5311.84231 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.05708 HOMO: -6.54978 LUMO: 2.00276 factor:1 | 1 (-0.84908) | -1 | -1 |
| G: -5311.84231 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.11439 HOMO: -6.62325 LUMO: 2.05990 factor:1 | 1 (-0.90638) | 1 | 1 |
| G: -5311.84231 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.17559 HOMO: -6.86271 LUMO: 2.14970 factor:1 | 1 (-0.96758) | 1 | 1 |
| G: -5311.84231 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.18280 HOMO: -6.77564 LUMO: 2.25855 factor:1 | 1 (-0.97479) | 1 | -1 |
| G: -5311.84231 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.11270 HOMO: -6.71305 LUMO: 1.94561 factor:1 | 1 (-0.90470) | 1 | -1 |
| G: -5311.84231 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.90410 HOMO: -6.75659 LUMO: 1.94561 factor:1 | 1 (-0.69609) | 1 | -1 |
| G: -5311.84231 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.87038 HOMO: -6.94979 LUMO: 2.33474 factor:1 | 1 (-0.66238) | 1 | -1 |
| G: -5311.84231 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.75283 HOMO: -6.85727 LUMO: 2.50345 factor:1 | 1 (-0.54483) | 1 | -1 |
| G: -5311.84231 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.90707 HOMO: -6.87360 LUMO: 2.43270 factor:1 | 1 (-0.69906) | 1 | -1 |
| G: -5311.84231 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.67103 HOMO: -6.57427 LUMO: 2.46807 factor:1 | 1 (-0.46303) | 1 | -1 |
| G: -5311.84231 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.89659 HOMO: -7.16204 LUMO: 2.15242 factor:1 | 1 (-0.68858) | 1 | 1 |
| G: -5311.84231 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.69893 HOMO: -6.62869 LUMO: 2.11432 factor:1 | 1 (-0.49092) | 1 | -1 |
| G: -5311.84231 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.93077 HOMO: -7.05591 LUMO: 2.26671 factor:1 | 1 (-0.72276) | 1 | -1 |
| G: -5311.84231 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.89904 HOMO: -7.13483 LUMO: 1.47758 factor:1 | 1 (-0.69103) | -1 | -1 |
| G: -5311.84231 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.77642 HOMO: -6.72938 LUMO: 1.57282 factor:1 | 1 (-0.56842) | -1 | -1 |
| G: -5311.84231 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.86100 HOMO: -6.17426 LUMO: 1.81228 factor:1 | 1 (-0.65299) | -1 | -1 |
| G: -5311.84231 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.59930 HOMO: -6.65318 LUMO: 1.93473 factor:1 | 1 (-0.39130) | 1 | -1 |
| G: -5311.84231 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.92663 HOMO: -6.18515 LUMO: 2.01364 factor:1 | 1 (-0.71863) | -1 | -1 |
| G: -5311.84231 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.68611 HOMO: -7.05591 LUMO: 2.13337 factor:1 | 1 (-0.47810) | 1 | 1 |
| G: -5311.84231 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.55683 HOMO: -6.90897 LUMO: 2.29664 factor:1 | 1 (-0.34882) | 1 | -1 |
| G: -5311.84231 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.51397 HOMO: -7.11034 LUMO: 2.17147 factor:1 | 1 (-0.30596) | 1 | 1 |
| G: -5311.84231 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.76355 HOMO: -6.82734 LUMO: 2.26671 factor:1 | 1 (-0.55555) | 1 | 1 |
| G: -5311.84231 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.57638 HOMO: -6.34842 LUMO: 2.34562 factor:1 | 1 (-1.36838) | -1 | -1 |
| G: -5311.84231 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.40958 HOMO: -6.62053 LUMO: 2.22861 factor:1 | 1 (-1.20157) | 1 | -1 |
| G: -5311.84231 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.54188 HOMO: -6.80557 LUMO: 2.07079 factor:1 | 1 (-1.33387) | 1 | -1 |
| G: -5311.84231 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.58384 HOMO: -6.60692 LUMO: 2.46263 factor:1 | 1 (-1.37583) | 1 | -1 |
| G: -5311.84231 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.70945 HOMO: -7.02054 LUMO: 2.08711 factor:1 | 1 (-1.50144) | 1 | -1 |
| G: -5311.84231 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.77786 HOMO: -6.78652 LUMO: 2.02453 factor:1 | 1 (-1.56985) | 1 | 1 |
| G: -5311.84231 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.55861 HOMO: -6.51168 LUMO: 2.06534 factor:1 | 1 (-1.35061) | -1 | -1 |
| G: -5311.84231 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.61418 HOMO: -6.50080 LUMO: 2.01636 factor:1 | 1 (-1.40618) | -1 | -1 |
| G: -5311.84231 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.50438 HOMO: -6.54434 LUMO: 1.84493 factor:1 | 1 (-1.29638) | -1 | -1 |
| G: -5311.84231 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.91176 HOMO: -6.47087 LUMO: 1.76330 factor:1 | 1 (-1.70376) | -1 | -1 |
| G: -5311.84231 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.48765 HOMO: -6.78924 LUMO: 2.39460 factor:1 | 1 (-1.27964) | 1 | 1 |
| G: -5311.84231 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.36862 HOMO: -6.59876 LUMO: 1.84493 factor:1 | 1 (-1.16062) | 1 | 1 |
| G: -5311.84231 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.25153 HOMO: -6.41644 LUMO: 2.05174 factor:1 | 1 (-1.04353) | -1 | -1 |
| G: -5311.84231 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.34509 HOMO: -6.52257 LUMO: 2.11160 factor:1 | 1 (-1.13708) | -1 | -1 |
| G: -5311.84231 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.64632 HOMO: -6.90897 LUMO: 2.34018 factor:1 | 1 (-1.43831) | 1 | 1 |
| G: -5311.84231 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.79182 HOMO: -6.97428 LUMO: 1.86126 factor:1 | 1 (-1.58381) | 1 | 1 |
| G: -5311.84231 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.57162 HOMO: -7.13483 LUMO: 2.14698 factor:1 | 1 (-1.36362) | 1 | -1 |
| G: -5311.84231 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.62871 HOMO: -7.16748 LUMO: 2.31841 factor:1 | 1 (-1.42071) | 1 | 1 |
| G: -5311.84231 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.87715 HOMO: -6.87087 LUMO: 2.38916 factor:1 | 1 (-1.66915) | 1 | -1 |
| G: -5311.84231 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.87813 HOMO: -6.93074 LUMO: 2.42181 factor:1 | 1 (-1.67013) | 1 | -1 |
| G: -5311.84231 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.57652 HOMO: -6.90081 LUMO: 2.00276 factor:1 | 1 (-1.36852) | 1 | -1 |
| G: -5311.84231 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.59940 HOMO: -6.99333 LUMO: 2.03541 factor:1 | 1 (-1.39140) | 1 | 1 |
| G: -5311.84231 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.48025 HOMO: -6.89264 LUMO: 1.57554 factor:1 | 1 (-1.27224) | -1 | -1 |
| G: -5311.84231 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.39891 HOMO: -6.48175 LUMO: 1.85854 factor:1 | 1 (-1.19091) | -1 | -1 |
| G: -5311.84231 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.41015 HOMO: -6.69400 LUMO: 1.62452 factor:1 | 1 (-1.20214) | 1 | 1 |
| G: -5311.84231 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.72392 HOMO: -6.50896 LUMO: 1.88303 factor:1 | 1 (-1.51592) | -1 | -1 |
| G: -5311.84231 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.55203 HOMO: -6.60420 LUMO: 2.05990 factor:1 | 1 (-1.34402) | 1 | 1 |
| G: -5311.84231 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.55497 HOMO: -7.14299 LUMO: 2.07351 factor:1 | 1 (-1.34696) | 1 | 1 |
| G: -5311.84231 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11578.15727 HOMO: -7.06408 LUMO: 1.81228 factor:1 | 1 (-1.94926) | 1 | 1 |
| G: -5311.84231 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11578.38769 HOMO: -6.67495 LUMO: 1.79595 factor:1 | 1 (-2.17969) | 1 | 1 |
| G: -5311.84231 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11578.98297 HOMO: -6.45182 LUMO: 2.15786 factor:1 | 1 (-2.77496) | -1 | -1 |
| G: -5311.84231 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.97255 HOMO: -6.93346 LUMO: 2.45719 factor:1 | 1 (-1.76455) | 1 | 1 |
| G: -5311.84231 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.96265 HOMO: -6.50080 LUMO: 2.08167 factor:1 | 1 (-1.75464) | -1 | -1 |
| G: -5311.84231 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11578.18861 HOMO: -6.83550 LUMO: -0.67484 factor:1 | 1 (-1.98061) | -1 | -1 |
| G: -5311.84231 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.99873 HOMO: -7.04231 LUMO: 0.54151 factor:1 | 1 (-1.79073) | -1 | -1 |
| G: -5311.84231 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.96820 HOMO: -6.79740 LUMO: 1.91296 factor:1 | 1 (-1.76020) | -1 | -1 |
| G: -5311.84231 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11578.19425 HOMO: -7.35796 LUMO: -1.04220 factor:1 | 1 (-1.98624) | -1 | -1 |
| G: -5311.84231 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.83141 HOMO: -6.62597 LUMO: -0.44082 factor:1 | 1 (-1.62340) | -1 | -1 |
| G: -5311.84231 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11578.98033 HOMO: -6.45182 LUMO: -0.20409 factor:1 | 1 (-2.77232) | -1 | -1 |
| G: -5311.84231 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11578.98218 HOMO: -6.51168 LUMO: -0.23130 factor:1 | 1 (-2.77417) | -1 | -1 |
| G: -5311.84231 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.79497 HOMO: -7.14027 LUMO: 0.49797 factor:1 | 1 (-1.58697) | -1 | -1 |
| G: -5311.84231 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11578.00496 HOMO: -7.55660 LUMO: 0.24762 factor:1 | 1 (-1.79696) | -1 | -1 |
| G: -5311.84231 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.93108 HOMO: -6.88992 LUMO: -0.64763 factor:1 | 1 (-1.72308) | -1 | -1 |
| G: -5311.84231 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.82882 HOMO: -6.72665 LUMO: -0.45987 factor:1 | 1 (-1.62082) | -1 | -1 |
| G: -5311.84231 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.58974 HOMO: -6.72121 LUMO: -0.58232 factor:1 | 1 (-1.38174) | -1 | -1 |
| G: -5311.84231 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11578.11101 HOMO: -7.26816 LUMO: 0.32926 factor:1 | 1 (-1.90300) | -1 | -1 |
| G: -5311.84231 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11578.38206 HOMO: -6.57155 LUMO: -0.53606 factor:1 | 1 (-2.17405) | -1 | -1 |
| G: -5311.84231 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11578.12611 HOMO: -6.50896 LUMO: -0.43810 factor:1 | 1 (-1.91810) | -1 | -1 |
| G: -5311.84231 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11578.10246 HOMO: -6.73210 LUMO: -0.51430 factor:1 | 1 (-1.89446) | -1 | -1 |
| G: -5311.84231 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.89930 HOMO: -6.77019 LUMO: -0.62858 factor:1 | 1 (-1.69130) | -1 | -1 |
| G: -5311.84231 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.80412 HOMO: -6.82462 LUMO: -0.67484 factor:1 | 1 (-0.59612) | -1 | -1 |
| G: -5311.84231 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.83515 HOMO: -6.79740 LUMO: -0.55511 factor:1 | 1 (-0.62714) | -1 | -1 |
| G: -5311.84231 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.02075 HOMO: -6.79740 LUMO: -0.67756 factor:1 | 1 (-0.81275) | -1 | -1 |
| G: -5311.84231 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.78886 HOMO: -6.75114 LUMO: -0.55239 factor:1 | 1 (-0.58085) | -1 | -1 |
| G: -5311.84231 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.73950 HOMO: -6.49536 LUMO: -0.25307 factor:1 | 1 (-0.53149) | -1 | -1 |
| G: -5311.84231 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.80244 HOMO: -6.48992 LUMO: -0.25034 factor:1 | 1 (-0.59443) | -1 | -1 |
| G: -5311.84231 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.59253 HOMO: -6.52801 LUMO: -0.28028 factor:1 | 1 (-0.38452) | -1 | -1 |
| G: -5311.84231 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.69710 HOMO: -7.22462 LUMO: 0.52518 factor:1 | 1 (-0.48910) | -1 | -1 |
| G: -5311.84231 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.88628 HOMO: -6.59332 LUMO: -0.27211 factor:1 | 1 (-0.67827) | -1 | -1 |
| G: -5311.84231 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.77851 HOMO: -6.57427 LUMO: -0.16871 factor:1 | 1 (-1.57051) | -1 | -1 |
| G: -5311.84231 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11578.60606 HOMO: -6.71033 LUMO: 1.59187 factor:1 | 1 (-2.39806) | -1 | -1 |
| G: -5311.84231 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.94219 HOMO: -6.72121 LUMO: 2.00004 factor:1 | 1 (-1.73418) | -1 | -1 |
| G: -5311.84231 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.83549 HOMO: -6.61509 LUMO: 1.55921 factor:1 | 1 (-1.62749) | -1 | -1 |
| G: -5311.84231 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.77712 HOMO: -6.55250 LUMO: 1.73064 factor:1 | 1 (-1.56912) | -1 | -1 |
| G: -5311.84231 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.57110 HOMO: -6.66135 LUMO: 2.02181 factor:1 | 1 (-1.36310) | -1 | -1 |
| G: -5311.84231 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.80442 HOMO: -6.84911 LUMO: 1.98099 factor:1 | 1 (-1.59641) | -1 | -1 |
| G: -5311.84231 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.61530 HOMO: -6.66679 LUMO: 1.98371 factor:1 | 1 (-1.40729) | -1 | -1 |
| G: -5311.84231 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.80771 HOMO: -6.67495 LUMO: 2.04085 factor:1 | 1 (-1.59970) | -1 | -1 |
| G: -5311.84231 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.65108 HOMO: -6.89809 LUMO: 1.95106 factor:1 | 1 (-1.44307) | -1 | -1 |
| G: -5311.84231 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.80096 HOMO: -6.50352 LUMO: 1.88847 factor:1 | 1 (-1.59295) | -1 | -1 |
| G: -5311.84231 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.76194 HOMO: -6.93618 LUMO: 2.00004 factor:1 | 1 (-1.55393) | -1 | -1 |
| G: -5311.84231 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.88070 HOMO: -6.50896 LUMO: 1.73609 factor:1 | 1 (-0.67269) | -1 | -1 |
| G: -5311.84231 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.90424 HOMO: -6.69672 LUMO: 2.37283 factor:1 | 1 (-0.69623) | -1 | -1 |
| G: -5311.84231 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.00598 HOMO: -6.65591 LUMO: 2.20684 factor:1 | 1 (-0.79797) | -1 | -1 |
| G: -5311.84231 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.12816 HOMO: -6.23957 LUMO: 1.78507 factor:1 | 1 (-0.92015) | -1 | -1 |
| G: -5311.84231 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.02026 HOMO: -6.35114 LUMO: 1.92112 factor:1 | 1 (-0.81226) | -1 | -1 |
| G: -5311.84231 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.92772 HOMO: -6.53617 LUMO: 1.75241 factor:1 | 1 (-0.71971) | -1 | -1 |
| G: -5311.84231 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.90870 HOMO: -6.60420 LUMO: 1.78779 factor:1 | 1 (-0.70069) | -1 | -1 |
| G: -5311.84231 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.04040 HOMO: -7.40422 LUMO: -0.97145 factor:1 | 1 (-0.83240) | -1 | -1 |
| G: -5311.84231 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.96747 HOMO: -6.80013 LUMO: -0.69117 factor:1 | 1 (-0.75947) | -1 | -1 |
| G: -5311.84231 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.68956 HOMO: -6.68040 LUMO: -0.47076 factor:1 | 1 (-0.48156) | -1 | -1 |
| G: -5311.84231 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.93128 HOMO: -7.20285 LUMO: -0.66124 factor:1 | 1 (-0.72328) | -1 | -1 |
| G: -5311.84231 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.76001 HOMO: -6.82734 LUMO: -0.60137 factor:1 | 1 (-0.55201) | -1 | -1 |
| G: -5311.84231 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.96421 HOMO: -7.18653 LUMO: 0.59321 factor:1 | 1 (-0.75620) | -1 | -1 |
| G: -5311.84231 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.01020 HOMO: -7.29265 LUMO: 0.48164 factor:1 | 1 (-0.80219) | -1 | -1 |
| G: -5311.84231 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.77836 HOMO: -6.63414 LUMO: -0.25034 factor:1 | 1 (-0.57035) | -1 | -1 |
| G: -5311.84231 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.00339 HOMO: -7.20285 LUMO: 0.53879 factor:1 | 1 (-0.79539) | -1 | -1 |
| G: -5311.84231 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.81721 HOMO: -6.46815 LUMO: -0.21769 factor:1 | 1 (-0.60921) | -1 | -1 |
| G: -5311.84231 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.98712 HOMO: -6.57971 LUMO: -0.18776 factor:1 | 1 (-0.77912) | -1 | -1 |
| G: -5311.84231 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.77871 HOMO: -6.90897 LUMO: 1.91296 factor:1 | 1 (-0.57070) | -1 | -1 |
| G: -5311.84231 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.09684 HOMO: -6.67495 LUMO: 2.04358 factor:1 | 1 (-0.88883) | -1 | -1 |
| G: -5311.84231 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.80837 HOMO: -6.94162 LUMO: 1.73881 factor:1 | 1 (-0.60036) | -1 | -1 |
| G: -5311.84231 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.56178 HOMO: -6.73482 LUMO: 1.95922 factor:1 | 1 (-0.35378) | -1 | -1 |
| G: -5311.84231 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.81928 HOMO: -6.70489 LUMO: 2.04358 factor:1 | 1 (-0.61128) | -1 | -1 |
| G: -5311.84231 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.04212 HOMO: -7.04231 LUMO: 1.79323 factor:1 | 1 (-0.83411) | -1 | -1 |
| G: -5311.84231 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.84208 HOMO: -6.68584 LUMO: 1.60275 factor:1 | 1 (-0.63408) | -1 | -1 |
| G: -5311.84231 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.93322 HOMO: -6.40556 LUMO: 1.45581 factor:1 | 1 (-0.72521) | -1 | -1 |
| G: -5311.84231 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.72227 HOMO: -6.94979 LUMO: 2.16603 factor:1 | 1 (-0.51427) | -1 | -1 |
| G: -5311.84231 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.04337 HOMO: -6.84911 LUMO: 1.89935 factor:1 | 1 (-0.83536) | -1 | -1 |
| G: -5311.84231 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.83278 HOMO: -6.22052 LUMO: 1.57282 factor:1 | 1 (-0.62477) | -1 | -1 |
| G: -5311.84231 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.79207 HOMO: -6.51168 LUMO: 2.10072 factor:1 | 1 (-0.58407) | -1 | -1 |
| G: -5311.84231 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.51941 HOMO: -7.03686 LUMO: 2.12249 factor:1 | 1 (-0.31141) | -1 | -1 |
| G: -5311.84231 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.88617 HOMO: -6.84094 LUMO: 1.63268 factor:1 | 1 (-0.67816) | -1 | -1 |
| G: -5311.84231 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.62926 HOMO: -6.75387 LUMO: 1.72248 factor:1 | 1 (-0.42126) | -1 | -1 |
| G: -5311.84231 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.44537 HOMO: -6.86271 LUMO: 1.68711 factor:1 | 1 (-0.23736) | -1 | -1 |
| G: -5311.84231 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.64423 HOMO: -6.84094 LUMO: 2.02997 factor:1 | 1 (-0.43623) | -1 | -1 |
| G: -5311.84231 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.80597 HOMO: -6.80557 LUMO: 2.02725 factor:1 | 1 (-0.59797) | -1 | -1 |
| G: -5311.84231 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.78347 HOMO: -6.38651 LUMO: 1.53472 factor:1 | 1 (-0.57547) | -1 | -1 |
| G: -5311.84231 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.83830 HOMO: -7.51306 LUMO: 0.28572 factor:1 | 1 (-0.63030) | -1 | -1 |
| G: -5311.84231 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.88540 HOMO: -6.97972 LUMO: -0.74287 factor:1 | 1 (-0.67740) | -1 | -1 |
| G: -5311.84231 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.79493 HOMO: -6.83822 LUMO: -0.65852 factor:1 | 1 (-0.58692) | -1 | -1 |
| G: -5311.84231 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.75939 HOMO: -6.71305 LUMO: -0.49525 factor:1 | 1 (-0.55138) | -1 | -1 |
| G: -5311.84231 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.79498 HOMO: -6.60692 LUMO: -0.22313 factor:1 | 1 (-0.58698) | -1 | -1 |
| G: -5311.84231 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.94500 HOMO: -7.20013 LUMO: 0.55239 factor:1 | 1 (-0.73699) | -1 | -1 |
| G: -5311.84231 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.10780 HOMO: -6.60420 LUMO: -0.28028 factor:1 | 1 (-0.89980) | -1 | -1 |
| G: -5311.84231 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.96911 HOMO: -6.69128 LUMO: -0.30477 factor:1 | 1 (-0.76110) | -1 | -1 |
| G: -5311.84231 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.01485 HOMO: -6.65591 LUMO: -0.25579 factor:1 | 1 (-0.80684) | -1 | -1 |
| G: -5311.84231 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.94728 HOMO: -6.69128 LUMO: 1.70888 factor:1 | 1 (-0.73928) | -1 | -1 |
| G: -5311.84231 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.91156 HOMO: -6.50080 LUMO: 1.87759 factor:1 | 1 (-0.70355) | -1 | -1 |
| G: -5311.84231 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.79046 HOMO: -6.85727 LUMO: 1.99187 factor:1 | 1 (-0.58246) | -1 | -1 |
| G: -5311.84231 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.98707 HOMO: -6.58788 LUMO: 1.79051 factor:1 | 1 (-0.77906) | -1 | -1 |
| G: -5311.84231 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.87191 HOMO: -6.64230 LUMO: 2.16058 factor:1 | 1 (-0.66390) | -1 | -1 |
| G: -5311.84231 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.15814 HOMO: -6.58788 LUMO: 2.10616 factor:1 | 1 (-0.95014) | -1 | -1 |
| G: -5311.84231 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.97226 HOMO: -7.01782 LUMO: 2.13609 factor:1 | 1 (-0.76426) | -1 | -1 |
| G: -5311.84231 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.93123 HOMO: -6.31304 LUMO: 2.31841 factor:1 | 1 (-0.72322) | -1 | -1 |
| G: -5311.84231 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.89789 HOMO: -6.94979 LUMO: 2.07895 factor:1 | 1 (-0.68989) | -1 | -1 |
| G: -5311.84231 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.04990 HOMO: -6.88992 LUMO: 2.28031 factor:1 | 1 (-0.84189) | -1 | -1 |
| G: -5311.84231 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.78608 HOMO: -6.66407 LUMO: 2.07623 factor:1 | 1 (-0.57808) | -1 | -1 |
| G: -5311.84231 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.96845 HOMO: -6.52529 LUMO: 1.70071 factor:1 | 1 (-0.76045) | -1 | -1 |
| G: -5311.84231 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.77359 HOMO: -6.58788 LUMO: 1.57282 factor:1 | 1 (-0.56559) | -1 | -1 |
| G: -5311.84231 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.96737 HOMO: -6.55250 LUMO: 1.95378 factor:1 | 1 (-0.75936) | -1 | -1 |
| G: -5311.84231 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.77528 HOMO: -6.24773 LUMO: 1.77962 factor:1 | 1 (-0.56728) | -1 | -1 |
| G: -5311.84231 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.98138 HOMO: -6.31304 LUMO: 2.18507 factor:1 | 1 (-0.77337) | -1 | -1 |
| G: -5311.84231 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.81403 HOMO: -6.18243 LUMO: 2.01636 factor:1 | 1 (-0.60602) | -1 | -1 |
| G: -5311.84231 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.43704 HOMO: -6.99877 LUMO: 2.14970 factor:1 | 1 (-0.22904) | -1 | -1 |
| G: -5311.84231 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.65620 HOMO: -6.72665 LUMO: 2.07079 factor:1 | 1 (-0.44820) | -1 | -1 |
| G: -5311.84231 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.51533 HOMO: -6.36202 LUMO: 2.17419 factor:1 | 1 (-0.30733) | -1 | -1 |
| G: -5311.84231 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.85691 HOMO: -6.78652 LUMO: 2.05718 factor:1 | 1 (-0.64891) | -1 | -1 |
| G: -5311.84231 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.58203 HOMO: -6.87360 LUMO: 2.34290 factor:1 | 1 (-0.37402) | -1 | -1 |
| G: -5311.84231 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.54646 HOMO: -6.62053 LUMO: 1.89391 factor:1 | 1 (-0.33846) | -1 | -1 |
| G: -5311.84231 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.38580 HOMO: -6.58788 LUMO: 1.83133 factor:1 | 1 (-0.17780) | -1 | -1 |
| G: -5311.84231 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.73158 HOMO: -7.08584 LUMO: 1.91568 factor:1 | 1 (-0.52357) | 1 | 1 |
| G: -5311.84231 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.91675 HOMO: -6.56883 LUMO: 1.81228 factor:1 | 1 (-0.70875) | -1 | -1 |
| G: -5311.84231 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.91068 HOMO: -6.66135 LUMO: 1.92384 factor:1 | 1 (-0.70268) | -1 | -1 |
| G: -5311.84231 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.89278 HOMO: -6.64502 LUMO: 2.15786 factor:1 | 1 (-0.68477) | -1 | -1 |
| G: -5311.84231 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.01104 HOMO: -6.71305 LUMO: 1.91840 factor:1 | 1 (-0.80304) | -1 | -1 |
| G: -5311.84231 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.03980 HOMO: -6.44094 LUMO: 1.74425 factor:1 | 1 (-0.83180) | -1 | -1 |
| G: -5311.84231 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.92524 HOMO: -6.51985 LUMO: 1.84221 factor:1 | 1 (-0.71724) | -1 | -1 |
| G: -5311.84231 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.88745 HOMO: -6.63414 LUMO: -0.24762 factor:1 | 1 (-0.67944) | -1 | -1 |
| G: -5311.84231 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.84663 HOMO: -6.60420 LUMO: -0.22585 factor:1 | 1 (-0.63862) | -1 | -1 |
| G: -5311.84231 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.82842 HOMO: -7.19741 LUMO: 0.58232 factor:1 | 1 (-0.62042) | -1 | -1 |
| G: -5311.84231 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.72116 HOMO: -6.77019 LUMO: -0.56872 factor:1 | 1 (-0.51315) | -1 | -1 |
| G: -5311.84231 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.69435 HOMO: -7.46136 LUMO: 0.28844 factor:1 | 1 (-0.48635) | -1 | -1 |
| G: -5311.84231 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.71814 HOMO: -6.60420 LUMO: -0.54151 factor:1 | 1 (-0.51013) | -1 | -1 |
| G: -5311.84231 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.92380 HOMO: -6.53890 LUMO: -0.46531 factor:1 | 1 (-0.71580) | -1 | -1 |
| G: -5311.84231 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.67005 HOMO: -6.81645 LUMO: -0.57144 factor:1 | 1 (-1.46204) | -1 | -1 |
| G: -5311.84231 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.79258 HOMO: -7.48041 LUMO: 0.28572 factor:1 | 1 (-1.58457) | -1 | -1 |
| G: -5311.84231 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.86420 HOMO: -6.75659 LUMO: -0.45715 factor:1 | 1 (-1.65619) | -1 | -1 |
| G: -5311.84231 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.47829 HOMO: -6.66135 LUMO: -0.41906 factor:1 | 1 (-1.27028) | -1 | -1 |
| G: -5311.84231 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.43505 HOMO: -6.55794 LUMO: -0.27483 factor:1 | 1 (-1.22704) | -1 | -1 |
| G: -5311.84231 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.44961 HOMO: -7.07496 LUMO: -0.63403 factor:1 | 1 (-1.24160) | -1 | -1 |
| G: -5311.84231 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.43265 HOMO: -7.12394 LUMO: 0.53334 factor:1 | 1 (-1.22465) | -1 | -1 |
| G: -5311.84231 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.28158 HOMO: -6.53617 LUMO: -0.25579 factor:1 | 1 (-1.07357) | -1 | -1 |
| G: -5311.84231 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.62134 HOMO: -6.50896 LUMO: -0.25034 factor:1 | 1 (-1.41333) | -1 | -1 |
| G: -5311.84231 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.47763 HOMO: -7.17564 LUMO: -0.68573 factor:1 | 1 (-1.26963) | -1 | -1 |
| G: -5311.84231 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.59516 HOMO: -6.53617 LUMO: -0.30749 factor:1 | 1 (-1.38715) | -1 | -1 |
| G: -5311.84231 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11578.21272 HOMO: -6.55522 LUMO: -0.30749 factor:1 | 1 (-2.00472) | -1 | -1 |
| G: -5311.84231 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11578.00401 HOMO: -7.05591 LUMO: -0.71022 factor:1 | 1 (-1.79601) | -1 | -1 |
| G: -5311.84231 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11578.02303 HOMO: -7.17564 LUMO: -0.69933 factor:1 | 1 (-1.81503) | -1 | -1 |
| G: -5311.84231 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11578.83529 HOMO: -6.78380 LUMO: -0.67756 factor:1 | 1 (-2.62729) | -1 | -1 |
| G: -5311.84231 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11578.98079 HOMO: -6.62325 LUMO: 2.02725 factor:1 | 1 (-2.77279) | -1 | -1 |
| G: -5311.84231 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.97506 HOMO: -6.63414 LUMO: 1.91296 factor:1 | 1 (-1.76705) | -1 | -1 |
| G: -5311.84231 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11578.15620 HOMO: -6.83278 LUMO: 1.65717 factor:1 | 1 (-1.94820) | -1 | -1 |
| G: -5311.84231 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.79141 HOMO: -6.66407 LUMO: 1.95650 factor:1 | 1 (-1.58340) | -1 | -1 |
| G: -5311.84231 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11578.04156 HOMO: -6.61237 LUMO: 2.11432 factor:1 | 1 (-1.83356) | -1 | -1 |
| G: -5311.84231 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.78665 HOMO: -6.62053 LUMO: 2.09256 factor:1 | 1 (-1.57864) | -1 | -1 |
| G: -5311.84231 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.80286 HOMO: -6.78652 LUMO: 2.13609 factor:1 | 1 (-1.59486) | -1 | -1 |
| G: -5311.84231 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.73818 HOMO: -6.94707 LUMO: 1.81772 factor:1 | 1 (-1.53018) | -1 | -1 |
| G: -5311.84231 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.59813 HOMO: -6.85183 LUMO: 2.12793 factor:1 | 1 (-1.39012) | -1 | -1 |
| G: -5311.84231 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.75245 HOMO: -6.81101 LUMO: 1.83949 factor:1 | 1 (-0.54445) | -1 | -1 |
| G: -5311.84231 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.96494 HOMO: -6.98788 LUMO: 2.16058 factor:1 | 1 (-0.75694) | -1 | -1 |
| G: -5311.84231 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.84187 HOMO: -6.62869 LUMO: 2.00820 factor:1 | 1 (-0.63386) | -1 | -1 |
| G: -5311.84231 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.90619 HOMO: -6.34025 LUMO: 2.25855 factor:1 | 1 (-0.69819) | -1 | -1 |
| G: -5311.84231 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.92399 HOMO: -6.01372 LUMO: 2.01636 factor:1 | 1 (-0.71599) | -1 | -1 |
| G: -5311.84231 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.91158 HOMO: -6.89264 LUMO: 2.27487 factor:1 | 1 (-0.70358) | -1 | -1 |
| G: -5311.84231 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.82829 HOMO: -6.53073 LUMO: 2.20684 factor:1 | 1 (-0.62028) | -1 | -1 |
| G: -5311.84231 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.77049 HOMO: -6.83278 LUMO: 1.53744 factor:1 | 1 (-0.56249) | -1 | -1 |
| G: -5311.84231 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.73539 HOMO: -6.41917 LUMO: 1.82316 factor:1 | 1 (-0.52738) | -1 | -1 |
| G: -5311.84231 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.56192 HOMO: -6.56339 LUMO: 1.63813 factor:1 | 1 (-0.35391) | -1 | -1 |
| G: -5311.84231 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.92170 HOMO: -6.88992 LUMO: 1.65173 factor:1 | 1 (-0.71370) | -1 | -1 |
| G: -5311.84231 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.75297 HOMO: -6.63141 LUMO: 1.92112 factor:1 | 1 (-0.54496) | -1 | -1 |
| G: -5311.84231 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.69699 HOMO: -6.83822 LUMO: 1.88847 factor:1 | 1 (-0.48899) | -1 | -1 |
| G: -5311.84231 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.98160 HOMO: -6.84638 LUMO: 1.90480 factor:1 | 1 (-0.77359) | -1 | -1 |
| G: -5311.84231 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.72401 HOMO: -6.82462 LUMO: 1.70888 factor:1 | 1 (-0.51601) | -1 | -1 |
| G: -5311.84231 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.75727 HOMO: -6.82734 LUMO: 2.12521 factor:1 | 1 (-0.54926) | -1 | -1 |
| G: -5311.84231 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.85528 HOMO: -6.94435 LUMO: 1.87214 factor:1 | 1 (-0.64728) | -1 | -1 |
| G: -5311.84231 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.76763 HOMO: -6.98516 LUMO: 2.51433 factor:1 | 1 (-0.55963) | -1 | -1 |
| G: -5311.84231 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.92845 HOMO: -6.74026 LUMO: 2.15514 factor:1 | 1 (-0.72045) | -1 | -1 |
| G: -5311.84231 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.62467 HOMO: -6.93618 LUMO: 2.54426 factor:1 | 1 (-0.41666) | -1 | -1 |
| G: -5311.84231 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.77778 HOMO: -6.28583 LUMO: 2.53610 factor:1 | 1 (-0.56978) | -1 | -1 |
| G: -5311.84231 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.50012 HOMO: -6.56883 LUMO: 1.94834 factor:1 | 1 (-0.29211) | -1 | -1 |
| G: -5311.84231 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.82051 HOMO: -7.08584 LUMO: 1.99187 factor:1 | 1 (-0.61250) | 1 | 1 |
| G: -5311.84231 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.71103 HOMO: -6.19059 LUMO: 1.99732 factor:1 | 1 (-0.50303) | -1 | -1 |
| G: -5311.84231 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.78891 HOMO: -6.78108 LUMO: 2.03813 factor:1 | 1 (-0.58091) | -1 | -1 |
| G: -5311.84231 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.69014 HOMO: -6.82189 LUMO: 1.77418 factor:1 | 1 (-0.48213) | -1 | -1 |
| G: -5311.84231 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.82894 HOMO: -6.45454 LUMO: 1.78779 factor:1 | 1 (-0.62094) | -1 | -1 |
| G: -5311.84231 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.67944 HOMO: -6.84366 LUMO: 1.77690 factor:1 | 1 (-0.47144) | -1 | -1 |
| G: -5311.84231 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.68910 HOMO: -6.74026 LUMO: 1.67622 factor:1 | 1 (-0.48110) | -1 | -1 |
| G: -5311.84231 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.54450 HOMO: -6.76475 LUMO: 2.40277 factor:1 | 1 (-0.33650) | -1 | -1 |
| G: -5311.84231 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.59109 HOMO: -6.65863 LUMO: 1.86670 factor:1 | 1 (-0.38308) | -1 | -1 |
| G: -5311.84231 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.88883 HOMO: -6.50080 LUMO: 1.93201 factor:1 | 1 (-0.68083) | -1 | -1 |
| G: -5311.84231 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.73686 HOMO: -6.34842 LUMO: 1.70888 factor:1 | 1 (-0.52885) | -1 | -1 |
| G: -5311.84231 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.79438 HOMO: -6.60692 LUMO: 2.20140 factor:1 | 1 (-0.58638) | -1 | -1 |
| G: -5311.84231 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.79302 HOMO: -6.74026 LUMO: 2.14970 factor:1 | 1 (-0.58502) | -1 | -1 |
| G: -5311.84231 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11578.18801 HOMO: -6.63686 LUMO: 2.17419 factor:1 | 1 (-1.98001) | -1 | -1 |
| G: -5311.84231 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11578.97167 HOMO: -6.81917 LUMO: 2.10072 factor:1 | 1 (-2.76367) | -1 | -1 |
| G: -5311.84231 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.98662 HOMO: -6.92802 LUMO: 2.04358 factor:1 | 1 (-1.77862) | -1 | -1 |
| G: -5311.84231 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11578.13373 HOMO: -6.56067 LUMO: -0.47620 factor:1 | 1 (-1.92572) | -1 | -1 |
| G: -5311.84231 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11578.14733 HOMO: -6.56611 LUMO: -0.77008 factor:1 | 1 (-1.93933) | -1 | -1 |
| G: -5311.84231 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11578.00404 HOMO: -6.78380 LUMO: -0.64763 factor:1 | 1 (-1.79603) | -1 | -1 |
| G: -5311.84231 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.68978 HOMO: -6.51985 LUMO: -0.24490 factor:1 | 1 (-0.48178) | -1 | -1 |
| G: -5311.84231 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.74864 HOMO: -6.52529 LUMO: -0.27483 factor:1 | 1 (-0.54064) | -1 | -1 |
| G: -5311.84231 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.75269 HOMO: -7.10489 LUMO: -0.62586 factor:1 | 1 (-0.54469) | -1 | -1 |
| G: -5311.84231 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.55775 HOMO: -7.18108 LUMO: 0.48980 factor:1 | 1 (-0.34975) | -1 | -1 |
| G: -5311.84231 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.61917 HOMO: -7.14299 LUMO: -0.63947 factor:1 | 1 (-0.41116) | -1 | -1 |
| G: -5311.84231 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.43552 HOMO: -6.70761 LUMO: -0.54423 factor:1 | 1 (-0.22751) | -1 | -1 |
| G: -5311.84231 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.42877 HOMO: -7.32258 LUMO: -1.03675 factor:1 | 1 (-0.22077) | -1 | -1 |
| G: -5311.84231 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.81506 HOMO: -6.65046 LUMO: -0.41361 factor:1 | 1 (-0.60706) | -1 | -1 |
| G: -5311.84231 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.65373 HOMO: -6.76475 LUMO: -0.60137 factor:1 | 1 (-0.44572) | -1 | -1 |
| G: -5311.84231 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.64442 HOMO: -6.77836 LUMO: -0.54423 factor:1 | 1 (-0.43642) | -1 | -1 |
| G: -5311.84231 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.74826 HOMO: -7.52395 LUMO: 0.26395 factor:1 | 1 (-0.54025) | -1 | -1 |
| G: -5311.84231 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11578.46035 HOMO: -6.93890 LUMO: -0.72382 factor:1 | 1 (-2.25234) | -1 | -1 |
| G: -5311.84231 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.67075 HOMO: -6.72938 LUMO: -0.47348 factor:1 | 1 (-1.46275) | -1 | -1 |
| G: -5311.84231 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.71456 HOMO: -6.66951 LUMO: -0.40817 factor:1 | 1 (-1.50656) | -1 | -1 |
| G: -5311.84231 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.74607 HOMO: -6.60420 LUMO: -0.19320 factor:1 | 1 (-1.53807) | -1 | -1 |
| G: -5311.84231 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.74722 HOMO: -6.67495 LUMO: -0.27211 factor:1 | 1 (-1.53921) | -1 | -1 |
| G: -5311.84231 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.60368 HOMO: -7.23823 LUMO: -0.62858 factor:1 | 1 (-1.39567) | -1 | -1 |
| G: -5311.84231 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.80047 HOMO: -7.27088 LUMO: 0.53334 factor:1 | 1 (-1.59246) | -1 | -1 |
| G: -5750.43323 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12013.72478 HOMO: -7.20013 LUMO: 0.59049 factor:1 | -1 (1.07414) | -1 | -1 |
| G: -5750.43323 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12013.27470 HOMO: -6.60148 LUMO: -0.20953 factor:1 | -1 (1.52422) | -1 | -1 |
| G: -5750.43323 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12013.53392 HOMO: -6.69400 LUMO: -0.51974 factor:1 | -1 (1.26500) | -1 | -1 |
| G: -5750.43323 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12013.38314 HOMO: -7.40422 LUMO: -0.98777 factor:1 | -1 (1.41578) | -1 | -1 |
| G: -5750.43323 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12013.67523 HOMO: -6.88176 LUMO: -0.71022 factor:1 | -1 (1.12369) | -1 | -1 |
| G: -5750.43323 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12013.25584 HOMO: -6.86271 LUMO: -0.59321 factor:1 | -1 (1.54308) | -1 | -1 |
| G: -5750.43323 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12013.45228 HOMO: -6.73754 LUMO: -0.55239 factor:1 | -1 (1.34664) | -1 | -1 |
| G: -5750.43323 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12013.62703 HOMO: -6.71033 LUMO: 1.57010 factor:1 | -1 (1.17189) | -1 | -1 |
| G: -5750.43323 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12013.41432 HOMO: -6.69672 LUMO: 1.68711 factor:1 | -1 (1.38460) | -1 | -1 |
| G: -5750.43323 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12013.48197 HOMO: -6.67495 LUMO: 2.03813 factor:1 | -1 (1.31695) | -1 | -1 |
| G: -5750.43323 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12013.48154 HOMO: -6.54434 LUMO: 1.83677 factor:1 | -1 (1.31738) | -1 | -1 |
| G: -5750.43323 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12013.64913 HOMO: -6.57155 LUMO: 1.77146 factor:1 | -1 (1.14979) | -1 | -1 |
| G: -5750.43323 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12013.36485 HOMO: -6.76747 LUMO: 1.87759 factor:1 | -1 (1.43407) | -1 | -1 |
| G: -5750.43323 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12013.46766 HOMO: -6.58243 LUMO: 1.61364 factor:1 | -1 (1.33126) | -1 | -1 |
| G: -5750.43323 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12013.28654 HOMO: -6.61781 LUMO: 2.13881 factor:1 | -1 (1.51238) | -1 | -1 |
| G: -5750.43323 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12013.39171 HOMO: -6.62597 LUMO: 2.00276 factor:1 | -1 (1.40721) | -1 | -1 |
| G: -5750.43323 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12013.26161 HOMO: -7.01237 LUMO: 1.95922 factor:1 | -1 (1.53731) | -1 | -1 |
| G: -5750.43323 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12013.42088 HOMO: -7.03959 LUMO: 2.16875 factor:1 | -1 (1.37804) | -1 | -1 |
| G: -5750.43323 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12013.18512 HOMO: -6.83278 LUMO: 1.91296 factor:1 | -1 (1.61380) | -1 | -1 |
| G: -5750.43323 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12013.29250 HOMO: -6.40012 LUMO: 1.95650 factor:1 | -1 (1.50642) | -1 | -1 |
| G: -5750.43323 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12013.49680 HOMO: -6.50080 LUMO: 1.73337 factor:1 | -1 (1.30212) | -1 | -1 |
| G: -5750.43323 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12013.10254 HOMO: -6.95795 LUMO: 2.28848 factor:1 | -1 (1.69639) | -1 | -1 |
| G: -5750.43323 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12013.38031 HOMO: -6.63686 LUMO: 2.20140 factor:1 | -1 (1.41861) | -1 | -1 |
| G: -5750.43323 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12013.53158 HOMO: -6.57427 LUMO: 1.87214 factor:1 | -1 (1.26734) | -1 | -1 |
| G: -5750.43323 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12013.43694 HOMO: -6.38379 LUMO: 2.32113 factor:1 | -1 (1.36198) | -1 | -1 |
| G: -5750.43323 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12013.25133 HOMO: -6.63958 LUMO: 2.04902 factor:1 | -1 (1.54759) | -1 | -1 |
| G: -5750.43323 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12013.36219 HOMO: -6.70216 LUMO: 1.93201 factor:1 | -1 (1.43673) | -1 | -1 |
| G: -5750.43323 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12013.53196 HOMO: -6.80557 LUMO: 2.23678 factor:1 | -1 (1.26696) | -1 | -1 |
| G: -5750.43323 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12013.52758 HOMO: -6.72938 LUMO: 2.28304 factor:1 | -1 (1.27134) | -1 | -1 |
| G: -5750.43323 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12013.32118 HOMO: -6.56067 LUMO: 1.66806 factor:1 | -1 (1.47774) | -1 | -1 |
| G: -5750.43323 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12013.22496 HOMO: -6.95523 LUMO: 2.33474 factor:1 | -1 (1.57396) | -1 | -1 |
| G: -5750.43323 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12013.33849 HOMO: -6.59876 LUMO: 2.30480 factor:1 | -1 (1.46044) | -1 | -1 |
| G: -5750.43323 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12013.45334 HOMO: -6.87360 LUMO: 1.75786 factor:1 | -1 (1.34558) | -1 | -1 |
| G: -5750.43323 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12013.39250 HOMO: -7.06408 LUMO: 1.99187 factor:1 | -1 (1.40642) | 1 | 1 |
| G: -5750.43323 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12013.19067 HOMO: -6.95795 LUMO: 1.88847 factor:1 | -1 (1.60825) | -1 | -1 |
| G: -5750.43323 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12013.40246 HOMO: -6.85455 LUMO: 1.63813 factor:1 | -1 (1.39646) | -1 | -1 |
| G: -5750.43323 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12013.31742 HOMO: -7.09129 LUMO: 2.31569 factor:1 | -1 (1.48150) | 1 | 1 |
| G: -5750.43323 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12013.41990 HOMO: -6.91441 LUMO: 1.68983 factor:1 | -1 (1.37902) | -1 | -1 |
| G: -5750.43323 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12013.34747 HOMO: -6.89809 LUMO: 2.23678 factor:1 | -1 (1.45146) | -1 | -1 |
| G: -5750.43323 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12014.97879 HOMO: -6.78652 LUMO: 1.98371 factor:1 | 1 (-0.17987) | -1 | -1 |
| G: -5750.43323 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12015.76746 HOMO: -6.94707 LUMO: 2.23678 factor:1 | 1 (-0.96853) | -1 | -1 |
| G: -5750.43323 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12016.10610 HOMO: -7.07224 LUMO: 2.13337 factor:1 | 1 (-1.30718) | 1 | 1 |
| G: -5750.43323 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12015.50827 HOMO: -6.94979 LUMO: 2.28031 factor:1 | 1 (-0.70935) | -1 | -1 |
| G: -5750.43323 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12015.57760 HOMO: -6.60965 LUMO: 2.20412 factor:1 | 1 (-0.77868) | -1 | -1 |
| G: -5750.43323 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12015.71679 HOMO: -6.87360 LUMO: 2.40277 factor:1 | 1 (-0.91787) | -1 | -1 |
| G: -5750.43323 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12015.74005 HOMO: -6.92802 LUMO: 1.89663 factor:1 | 1 (-0.94113) | -1 | -1 |
| G: -5750.43323 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12015.81333 HOMO: -6.88448 LUMO: 2.02725 factor:1 | 1 (-1.01441) | -1 | -1 |
| G: -5750.43323 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12015.70209 HOMO: -6.69128 LUMO: 1.55105 factor:1 | 1 (-0.90317) | -1 | -1 |
| G: -5750.43323 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12015.56625 HOMO: -6.54978 LUMO: 1.93201 factor:1 | 1 (-0.76733) | -1 | -1 |
| G: -5750.43323 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12015.65711 HOMO: -6.19331 LUMO: 1.46941 factor:1 | 1 (-0.85819) | -1 | -1 |
| G: -5750.43323 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12015.39801 HOMO: -6.55794 LUMO: 1.89663 factor:1 | 1 (-0.59909) | -1 | -1 |
| G: -5750.43323 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12014.93449 HOMO: -6.07630 LUMO: 1.94289 factor:1 | 1 (-0.13557) | -1 | -1 |
| G: -5750.43323 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12015.59700 HOMO: -7.46408 LUMO: 0.31565 factor:1 | 1 (-0.79808) | -1 | -1 |
| G: -5750.43323 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12015.69872 HOMO: -6.63958 LUMO: -0.61770 factor:1 | 1 (-0.89980) | -1 | -1 |
| G: -5750.43323 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12015.62909 HOMO: -6.81101 LUMO: -0.57960 factor:1 | 1 (-0.83016) | -1 | -1 |
| G: -5750.43323 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12015.55798 HOMO: -6.74298 LUMO: -0.57960 factor:1 | 1 (-0.75906) | -1 | -1 |
| G: -5750.43323 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12015.13395 HOMO: -6.63686 LUMO: -0.42994 factor:1 | 1 (-0.33503) | -1 | -1 |
| G: -5750.43323 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12013.52439 HOMO: -6.60965 LUMO: -0.41089 factor:1 | -1 (1.27453) | -1 | -1 |
| G: -5750.43323 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12015.21857 HOMO: -6.60692 LUMO: -0.80274 factor:1 | 1 (-0.41965) | -1 | -1 |
| G: -5750.43323 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12014.50041 HOMO: -6.58788 LUMO: -0.78097 factor:1 | -1 (0.29851) | -1 | -1 |
| G: -5750.43323 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12015.11830 HOMO: -6.67767 LUMO: -0.48436 factor:1 | 1 (-0.31938) | -1 | -1 |
| G: -5750.43323 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12013.50605 HOMO: -6.63141 LUMO: -0.40545 factor:1 | -1 (1.29287) | -1 | -1 |
| G: -5750.43323 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12013.26096 HOMO: -6.62053 LUMO: -0.83811 factor:1 | -1 (1.53796) | -1 | -1 |
| G: -5750.43323 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12013.65618 HOMO: -6.59604 LUMO: -0.35375 factor:1 | -1 (1.14274) | -1 | -1 |
| G: -5750.43323 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12016.15617 HOMO: -6.34297 LUMO: -0.39729 factor:1 | 1 (-1.35725) | -1 | -1 |
| G: -5750.43323 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12015.68604 HOMO: -6.67223 LUMO: 1.97827 factor:1 | 1 (-0.88712) | -1 | -1 |
| G: -5750.43323 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12015.65379 HOMO: -6.40012 LUMO: 1.89935 factor:1 | 1 (-0.85487) | -1 | -1 |
| G: -5750.43323 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12015.18143 HOMO: -6.74842 LUMO: 1.97283 factor:1 | 1 (-0.38251) | -1 | -1 |
| G: -5750.43323 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12013.37549 HOMO: -6.76747 LUMO: 2.17147 factor:1 | -1 (1.42343) | -1 | -1 |
| G: -5750.43323 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12015.62130 HOMO: -6.72121 LUMO: 1.55649 factor:1 | 1 (-0.82238) | -1 | -1 |
| G: -5750.43323 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12015.65249 HOMO: -6.97700 LUMO: 2.04085 factor:1 | 1 (-0.85357) | -1 | -1 |
| G: -5750.43323 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12015.66841 HOMO: -7.06680 LUMO: 2.04085 factor:1 | 1 (-0.86949) | 1 | 1 |
| G: -5750.43323 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12015.01816 HOMO: -7.09673 LUMO: 2.35106 factor:1 | 1 (-0.21924) | 1 | 1 |
| G: -5750.43323 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12013.50254 HOMO: -6.83006 LUMO: 2.14970 factor:1 | -1 (1.29638) | -1 | -1 |
| G: -5750.43323 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12013.35767 HOMO: -6.72665 LUMO: 2.20140 factor:1 | -1 (1.44125) | -1 | -1 |
| G: -5750.43323 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12015.32013 HOMO: -6.77291 LUMO: 2.34562 factor:1 | 1 (-0.52121) | -1 | -1 |
| G: -5750.43323 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12015.27264 HOMO: -6.73754 LUMO: 2.00276 factor:1 | 1 (-0.47372) | -1 | -1 |
| G: -5750.43323 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12013.92671 HOMO: -7.04231 LUMO: 1.92112 factor:1 | -1 (0.87221) | -1 | -1 |
| G: -5750.43323 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12013.64287 HOMO: -6.83822 LUMO: 1.72248 factor:1 | -1 (1.15605) | -1 | -1 |
| G: -5750.43323 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12013.57381 HOMO: -6.57971 LUMO: 2.16603 factor:1 | -1 (1.22511) | -1 | -1 |
| G: -5750.43323 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12013.76135 HOMO: -6.80013 LUMO: 1.88575 factor:1 | -1 (1.03757) | -1 | -1 |
| G: -5750.43323 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12013.69727 HOMO: -6.93618 LUMO: 2.18235 factor:1 | -1 (1.10165) | -1 | -1 |
| G: -5750.43323 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12015.75306 HOMO: -6.54706 LUMO: 1.91024 factor:1 | 1 (-0.95414) | -1 | -1 |
| G: -5750.43323 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12015.61937 HOMO: -7.06952 LUMO: 2.18507 factor:1 | 1 (-0.82045) | 1 | 1 |
| G: -5750.43323 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12015.90806 HOMO: -7.05047 LUMO: 1.82044 factor:1 | 1 (-1.10914) | -1 | -1 |
| G: -5750.43323 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12014.47353 HOMO: -6.87632 LUMO: 1.92657 factor:1 | -1 (0.32539) | -1 | -1 |
| G: -5750.43323 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12015.43379 HOMO: -6.58788 LUMO: 1.91568 factor:1 | 1 (-0.63487) | -1 | -1 |
| G: -5750.43323 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12015.65026 HOMO: -7.17292 LUMO: 1.90752 factor:1 | 1 (-0.85134) | 1 | 1 |
| G: -5750.43323 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12015.71921 HOMO: -6.93890 LUMO: 1.80684 factor:1 | 1 (-0.92029) | -1 | -1 |
| G: -5750.43323 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12015.58949 HOMO: -7.10761 LUMO: 2.20956 factor:1 | 1 (-0.79057) | 1 | 1 |
| G: -5750.43323 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12015.44750 HOMO: -6.85727 LUMO: 2.13609 factor:1 | 1 (-0.64858) | -1 | -1 |
| G: -5750.43323 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12013.45511 HOMO: -6.64502 LUMO: 1.38506 factor:1 | -1 (1.34381) | -1 | -1 |
| G: -5750.43323 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12015.65053 HOMO: -6.87360 LUMO: 1.15648 factor:1 | 1 (-0.85161) | -1 | -1 |
| G: -5750.43323 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12015.68419 HOMO: -6.67223 LUMO: 2.07351 factor:1 | 1 (-0.88527) | -1 | -1 |
| G: -5750.43323 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12015.35371 HOMO: -6.29671 LUMO: 2.43270 factor:1 | 1 (-0.55479) | -1 | -1 |
| G: -5750.43323 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12013.68320 HOMO: -6.90897 LUMO: 2.28848 factor:1 | -1 (1.11572) | -1 | -1 |
| G: -5750.43323 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12015.51316 HOMO: -7.04231 LUMO: 1.70071 factor:1 | 1 (-0.71424) | -1 | -1 |
| G: -5750.43323 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12014.21194 HOMO: -6.69944 LUMO: 1.94834 factor:1 | -1 (0.58698) | -1 | -1 |
| G: -5750.43323 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12013.55844 HOMO: -6.56067 LUMO: 2.20956 factor:1 | -1 (1.24049) | -1 | -1 |
| G: -5750.43323 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12015.18780 HOMO: -6.65046 LUMO: 2.06807 factor:1 | 1 (-0.38888) | -1 | -1 |
| G: -5750.43323 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12016.04093 HOMO: -7.08584 LUMO: 1.98915 factor:1 | 1 (-1.24201) | 1 | 1 |
| G: -5750.43323 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12015.46095 HOMO: -6.69400 LUMO: 2.09256 factor:1 | 1 (-0.66203) | -1 | -1 |
| G: -5750.43323 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12015.46957 HOMO: -6.62869 LUMO: 2.16331 factor:1 | 1 (-0.67065) | -1 | -1 |
| G: -5750.43323 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12015.59330 HOMO: -6.85183 LUMO: 2.16058 factor:1 | 1 (-0.79438) | -1 | -1 |
| G: -5750.43323 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12015.55651 HOMO: -6.54706 LUMO: 1.92384 factor:1 | 1 (-0.75759) | -1 | -1 |
| G: -5750.43323 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12015.56204 HOMO: -6.84366 LUMO: 2.48984 factor:1 | 1 (-0.76312) | -1 | -1 |
| G: -5750.43323 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12015.65573 HOMO: -6.77291 LUMO: 2.46263 factor:1 | 1 (-0.85680) | -1 | -1 |
| G: -5750.43323 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12015.61371 HOMO: -7.01782 LUMO: 2.31025 factor:1 | 1 (-0.81479) | -1 | -1 |
| G: -5750.43323 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12014.90211 HOMO: -6.94707 LUMO: 2.29664 factor:1 | 1 (-0.10319) | -1 | -1 |
| G: -5750.43323 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12015.26551 HOMO: -6.64230 LUMO: 1.97283 factor:1 | 1 (-0.46659) | -1 | -1 |
| G: -5750.43323 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12013.24624 HOMO: -6.47359 LUMO: 2.20412 factor:1 | -1 (1.55268) | -1 | -1 |
| G: -5750.43323 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12015.24274 HOMO: -6.90625 LUMO: 1.92384 factor:1 | 1 (-0.44382) | -1 | -1 |
| G: -5750.43323 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12015.32878 HOMO: -7.17020 LUMO: 2.06807 factor:1 | 1 (-0.52986) | 1 | 1 |
| G: -5750.43323 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12013.53849 HOMO: -6.65046 LUMO: 2.20956 factor:1 | -1 (1.26043) | -1 | -1 |
| G: -5750.43323 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12015.21569 HOMO: -7.07496 LUMO: 1.82861 factor:1 | 1 (-0.41677) | 1 | 1 |
| G: -5750.43323 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12015.47529 HOMO: -6.83006 LUMO: 2.14970 factor:1 | 1 (-0.67637) | -1 | -1 |
| G: -5750.43323 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12014.67944 HOMO: -6.92802 LUMO: 1.99187 factor:1 | -1 (0.11949) | -1 | -1 |
| G: -5750.43323 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12014.44691 HOMO: -6.69672 LUMO: 2.36739 factor:1 | -1 (0.35201) | -1 | -1 |
| G: -5750.43323 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12014.46422 HOMO: -7.13755 LUMO: 2.00276 factor:1 | -1 (0.33470) | 1 | 1 |
| G: -5750.43323 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12014.36400 HOMO: -6.92530 LUMO: 2.25582 factor:1 | -1 (0.43492) | -1 | -1 |
| G: -5750.43323 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12015.62740 HOMO: -6.77564 LUMO: 1.97827 factor:1 | 1 (-0.82848) | -1 | -1 |
| G: -5750.43323 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12015.36157 HOMO: -6.87904 LUMO: 1.60003 factor:1 | 1 (-0.56265) | -1 | -1 |
| G: -5750.43323 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12015.33474 HOMO: -6.62869 LUMO: 1.90480 factor:1 | 1 (-0.53582) | -1 | -1 |
| G: -5750.43323 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12015.09242 HOMO: -6.71033 LUMO: 1.54833 factor:1 | 1 (-0.29350) | -1 | -1 |
| G: -5750.43323 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12015.28894 HOMO: -6.74298 LUMO: 1.47486 factor:1 | 1 (-0.49002) | -1 | -1 |
| G: -5750.43323 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12014.25660 HOMO: -6.77019 LUMO: 1.90480 factor:1 | -1 (0.54232) | -1 | -1 |
| G: -5750.43323 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12015.54152 HOMO: -6.70489 LUMO: 1.99459 factor:1 | 1 (-0.74260) | -1 | -1 |