乙二醇作为反应物的反应表19-8

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: -5312.08863 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.38057 HOMO: -6.91169 LUMO: -0.53879 factor:1 | 1 (-0.92625) | -1 | -1 |
| G: -5312.08863 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.16176 HOMO: -7.29809 LUMO: 2.83543 factor:1 | 1 (-0.70744) | 1 | -1 |
| G: -5312.08863 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.94481 HOMO: -6.86543 LUMO: -0.70205 factor:1 | 1 (-0.49049) | -1 | -1 |
| G: -5312.08863 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.86679 HOMO: -7.47769 LUMO: 0.31293 factor:1 | 1 (-0.41247) | -1 | -1 |
| G: -5312.08863 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.16906 HOMO: -6.63141 LUMO: -0.55511 factor:1 | 1 (-0.71473) | -1 | -1 |
| G: -5312.08863 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.93460 HOMO: -6.68856 LUMO: -0.30205 factor:1 | 1 (-0.48028) | -1 | -1 |
| G: -5312.08863 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.21706 HOMO: -7.22190 LUMO: 0.53334 factor:1 | 1 (-0.76274) | -1 | -1 |
| G: -5312.08863 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.88181 HOMO: -6.66407 LUMO: -0.27756 factor:1 | 1 (-0.42749) | -1 | -1 |
| G: -5312.08863 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.90274 HOMO: -7.15659 LUMO: -0.70205 factor:1 | 1 (-0.44842) | -1 | -1 |
| G: -5312.08863 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.03129 HOMO: -6.69400 LUMO: 1.67622 factor:1 | 1 (-0.57696) | -1 | -1 |
| G: -5312.08863 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.05471 HOMO: -6.60420 LUMO: 2.16058 factor:1 | 1 (-0.60039) | -1 | -1 |
| G: -5312.08863 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.27061 HOMO: -6.87087 LUMO: 1.88031 factor:1 | 1 (-0.81629) | -1 | -1 |
| G: -5312.08863 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.14631 HOMO: -6.60965 LUMO: -0.19864 factor:1 | 1 (-0.69199) | -1 | -1 |
| G: -5312.08863 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.00557 HOMO: -7.29265 LUMO: 0.52246 factor:1 | 1 (-0.55125) | -1 | -1 |
| G: -5312.08863 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.11578 HOMO: -6.86543 LUMO: -0.59593 factor:1 | 1 (-0.66145) | -1 | -1 |
| G: -5312.08863 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.31690 HOMO: -7.44504 LUMO: -1.01226 factor:1 | 1 (-0.86257) | -1 | -1 |
| G: -5312.08863 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.00252 HOMO: -6.92530 LUMO: -0.75103 factor:1 | 1 (-0.54820) | -1 | -1 |
| G: -5312.08863 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.12522 HOMO: -7.10489 LUMO: 2.20412 factor:1 | 1 (-0.67090) | 1 | 1 |
| G: -5312.08863 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.01020 HOMO: -6.58788 LUMO: 1.73881 factor:1 | 1 (-0.55587) | -1 | -1 |
| G: -5312.08863 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.08067 HOMO: -6.64502 LUMO: 1.70343 factor:1 | 1 (-0.62635) | -1 | -1 |
| G: -5312.08863 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.06127 HOMO: -6.73754 LUMO: 1.60819 factor:1 | 1 (-0.60695) | -1 | -1 |
| G: -5312.08863 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.15706 HOMO: -6.80829 LUMO: 2.45991 factor:1 | 1 (-0.70273) | -1 | -1 |
| G: -5312.08863 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.65244 HOMO: -6.91713 LUMO: 2.43814 factor:1 | 1 (-1.19812) | -1 | -1 |
| G: -5312.08863 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.76240 HOMO: -6.60692 LUMO: 1.93745 factor:1 | 1 (-1.30808) | -1 | -1 |
| G: -5312.08863 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.95296 HOMO: -6.26134 LUMO: 1.46125 factor:1 | 1 (-1.49864) | -1 | -1 |
| G: -5312.08863 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.53309 HOMO: -7.54028 LUMO: 0.25851 factor:1 | 1 (-1.07877) | -1 | -1 |
| G: -5312.08863 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.78809 HOMO: -6.97700 LUMO: -0.73471 factor:1 | 1 (-1.33377) | -1 | -1 |
| G: -5312.08863 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.64134 HOMO: -6.92258 LUMO: -0.70205 factor:1 | 1 (-1.18702) | -1 | -1 |
| G: -5312.08863 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11578.02616 HOMO: -6.83550 LUMO: -0.56872 factor:1 | 1 (-1.57184) | -1 | -1 |
| G: -5312.08863 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.81554 HOMO: -6.72121 LUMO: 1.89663 factor:1 | 1 (-1.36122) | -1 | -1 |
| G: -5312.08863 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.89647 HOMO: -6.73482 LUMO: 1.89935 factor:1 | 1 (-1.44215) | -1 | -1 |
| G: -5312.08863 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.96118 HOMO: -6.61781 LUMO: 1.86670 factor:1 | 1 (-1.50686) | -1 | -1 |
| G: -5312.08863 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.97621 HOMO: -7.01782 LUMO: 2.26399 factor:1 | 1 (-0.52189) | -1 | -1 |
| G: -5312.08863 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.02353 HOMO: -7.23551 LUMO: 2.09800 factor:1 | 1 (-0.56921) | 1 | 1 |
| G: -5312.08863 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.14419 HOMO: -7.13483 LUMO: 2.17963 factor:1 | 1 (-0.68986) | 1 | 1 |
| G: -5312.08863 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.08429 HOMO: -6.22869 LUMO: 2.01092 factor:1 | 1 (-0.62997) | -1 | -1 |
| G: -5312.08863 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.99433 HOMO: -6.80285 LUMO: 2.14970 factor:1 | 1 (-0.54001) | -1 | -1 |
| G: -5312.08863 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.78886 HOMO: -7.21102 LUMO: 2.33746 factor:1 | 1 (-0.33454) | 1 | 1 |
| G: -5312.08863 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.83689 HOMO: -6.39740 LUMO: 2.59597 factor:1 | 1 (-0.38256) | -1 | -1 |
| G: -5312.08863 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.91945 HOMO: -7.07768 LUMO: 2.48168 factor:1 | 1 (-0.46512) | 1 | 1 |
| G: -5312.08863 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.97485 HOMO: -7.11306 LUMO: 0.90614 factor:1 | 1 (-0.52053) | -1 | -1 |
| G: -5312.08863 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.14516 HOMO: -6.61781 LUMO: -2.46263 factor:1 | 1 (-0.69084) | -1 | -1 |
| G: -5312.08863 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.85101 HOMO: -6.96611 LUMO: 0.90614 factor:1 | 1 (-0.39669) | -1 | -1 |
| G: -5312.08863 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.75041 HOMO: -6.86271 LUMO: -1.14832 factor:1 | 1 (-0.29609) | -1 | -1 |
| G: -5312.08863 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.88045 HOMO: -6.72665 LUMO: 0.96873 factor:1 | 1 (-0.42613) | -1 | -1 |
| G: -5312.08863 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.78189 HOMO: -7.14571 LUMO: 1.05036 factor:1 | 1 (-0.32757) | -1 | -1 |
| G: -5312.08863 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.06329 HOMO: -7.14299 LUMO: 0.98777 factor:1 | 1 (-0.60896) | -1 | -1 |
| G: -5312.08863 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.90037 HOMO: -6.99333 LUMO: 1.05852 factor:1 | 1 (-0.44605) | -1 | -1 |
| G: -5312.08863 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.05787 HOMO: -6.78924 LUMO: -1.49935 factor:1 | 1 (-0.60355) | -1 | -1 |
| G: -5312.08863 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11578.95440 HOMO: -7.13755 LUMO: 0.94151 factor:1 | 1 (-2.50007) | -1 | -1 |
| G: -5312.08863 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11578.00401 HOMO: -6.72938 LUMO: -0.35375 factor:1 | 1 (-1.54969) | -1 | -1 |
| G: -5312.08863 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11578.22633 HOMO: -6.99061 LUMO: 0.82450 factor:1 | 1 (-1.77201) | -1 | -1 |
| G: -5312.08863 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11578.35074 HOMO: -6.75114 LUMO: -0.68028 factor:1 | 1 (-1.89642) | -1 | -1 |
| G: -5312.08863 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.72037 HOMO: -6.40556 LUMO: -0.42722 factor:1 | 1 (-0.26605) | -1 | -1 |
| G: -5312.08863 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.85237 HOMO: -7.18653 LUMO: 0.42178 factor:1 | 1 (-0.39805) | -1 | -1 |
| G: -5312.08863 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.97158 HOMO: -6.63958 LUMO: -0.71294 factor:1 | 1 (-0.51726) | -1 | -1 |
| G: -5312.08863 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.81248 HOMO: -6.63958 LUMO: -0.71022 factor:1 | 1 (-0.35816) | -1 | -1 |
| G: -5312.08863 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.69759 HOMO: -6.69672 LUMO: -0.72654 factor:1 | 1 (-0.24327) | -1 | -1 |
| G: -5312.08863 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11578.44543 HOMO: -6.56883 LUMO: -0.80274 factor:1 | 1 (-1.99111) | -1 | -1 |
| G: -5312.08863 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.65519 HOMO: -6.68584 LUMO: -0.56872 factor:1 | 1 (-1.20087) | -1 | -1 |
| G: -5312.08863 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.75337 HOMO: -6.59060 LUMO: -0.35647 factor:1 | 1 (-1.29904) | -1 | -1 |
| G: -5312.08863 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.83933 HOMO: -6.72121 LUMO: -0.71838 factor:1 | 1 (-1.38501) | -1 | -1 |
| G: -5312.08863 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.96779 HOMO: -6.57971 LUMO: -0.61498 factor:1 | 1 (-1.51347) | -1 | -1 |
| G: -5312.08863 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.95855 HOMO: -7.07496 LUMO: 0.50613 factor:1 | 1 (-0.50423) | -1 | -1 |
| G: -5312.08863 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.21649 HOMO: -7.14027 LUMO: 0.43266 factor:1 | 1 (-0.76216) | -1 | -1 |
| G: -5312.08863 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.91822 HOMO: -6.43277 LUMO: -0.44082 factor:1 | 1 (-0.46390) | -1 | -1 |
| G: -5312.08863 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.98994 HOMO: -6.79468 LUMO: 0.07619 factor:1 | 1 (-1.53562) | -1 | -1 |
| G: -5312.08863 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.99277 HOMO: -6.81917 LUMO: -2.57148 factor:1 | 1 (-1.53845) | -1 | -1 |
| G: -5312.08863 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.87527 HOMO: -6.71849 LUMO: 1.30615 factor:1 | 1 (-1.42095) | -1 | -1 |
| G: -5312.08863 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.86178 HOMO: -6.85455 LUMO: -0.63675 factor:1 | 1 (-1.40745) | -1 | -1 |
| G: -5312.08863 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.93106 HOMO: -6.73210 LUMO: -1.03131 factor:1 | 1 (-1.47673) | -1 | -1 |
| G: -5312.08863 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11578.52731 HOMO: -6.83550 LUMO: -0.58777 factor:1 | 1 (-2.07299) | -1 | -1 |
| G: -5312.08863 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.20008 HOMO: -6.53073 LUMO: -0.74287 factor:1 | 1 (-0.74576) | -1 | -1 |
| G: -5312.08863 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11578.21245 HOMO: -7.18381 LUMO: -0.92791 factor:1 | 1 (-1.75813) | -1 | -1 |
| G: -5312.08863 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11578.08701 HOMO: -6.49264 LUMO: -0.44627 factor:1 | 1 (-1.63268) | -1 | -1 |
| G: -5312.08863 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.99424 HOMO: -7.32803 LUMO: 0.41361 factor:1 | 1 (-1.53992) | -1 | -1 |
| G: -5312.08863 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.67342 HOMO: -6.53073 LUMO: -0.52790 factor:1 | 1 (-1.21910) | -1 | -1 |
| G: -5312.08863 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.91821 HOMO: -6.54978 LUMO: -0.53062 factor:1 | 1 (-1.46389) | -1 | -1 |
| G: -5312.08863 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11578.06709 HOMO: -6.56611 LUMO: -0.37824 factor:1 | 1 (-1.61276) | -1 | -1 |
| G: -5312.08863 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.82091 HOMO: -6.57155 LUMO: -0.64219 factor:1 | 1 (-1.36658) | -1 | -1 |
| G: -5312.08863 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.66515 HOMO: -7.08040 LUMO: 0.45715 factor:1 | 1 (-1.21083) | -1 | -1 |
| G: -5312.08863 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.37486 HOMO: -6.66679 LUMO: -0.75376 factor:1 | 1 (-0.92053) | -1 | -1 |
| G: -5312.08863 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.47339 HOMO: -6.83550 LUMO: -0.99322 factor:1 | 1 (-1.01907) | -1 | -1 |
| G: -5312.08863 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.45910 HOMO: -6.53345 LUMO: -0.29660 factor:1 | 1 (-1.00478) | -1 | -1 |
| G: -5312.08863 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.26756 HOMO: -6.65046 LUMO: 2.40549 factor:1 | 1 (-0.81324) | -1 | -1 |
| G: -5312.08863 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.88371 HOMO: -6.98788 LUMO: 2.01092 factor:1 | 1 (-1.42939) | -1 | -1 |
| G: -5312.08863 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.62332 HOMO: -6.61781 LUMO: 1.92384 factor:1 | 1 (-1.16900) | -1 | -1 |
| G: -5312.08863 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.62354 HOMO: -6.61237 LUMO: 2.06807 factor:1 | 1 (-1.16922) | -1 | -1 |
| G: -5312.08863 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.48607 HOMO: -6.59060 LUMO: 1.95106 factor:1 | 1 (-1.03175) | -1 | -1 |
| G: -5312.08863 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.54626 HOMO: -6.48175 LUMO: 1.72248 factor:1 | 1 (-1.09194) | -1 | -1 |
| G: -5312.08863 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.46640 HOMO: -6.84911 LUMO: 2.03541 factor:1 | 1 (-1.01207) | -1 | -1 |
| G: -5312.08863 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.40193 HOMO: -6.50624 LUMO: 2.17147 factor:1 | 1 (-0.94761) | -1 | -1 |
| G: -5312.08863 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: 2.08439 factor:1 | 1 (-0.72241) | -1 | -1 |
| G: -5312.08863 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.32386 HOMO: -6.96067 LUMO: 1.98099 factor:1 | 1 (-0.86954) | -1 | -1 |
| G: -5312.08863 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.29080 HOMO: -6.93618 LUMO: 1.85854 factor:1 | 1 (-0.83648) | -1 | -1 |
| G: -5312.08863 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.73803 HOMO: -6.71305 LUMO: -0.61226 factor:1 | 1 (-0.28371) | -1 | -1 |
| G: -5312.08863 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.10696 HOMO: -7.06408 LUMO: 0.80001 factor:1 | 1 (-0.65264) | -1 | -1 |
| G: -5312.08863 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.27080 HOMO: -6.52257 LUMO: 0.99049 factor:1 | 1 (-0.81648) | -1 | -1 |
| G: -5312.08863 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.31456 HOMO: -6.84638 LUMO: 1.10750 factor:1 | 1 (-0.86023) | -1 | -1 |
| G: -5312.08863 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.44906 HOMO: -6.85455 LUMO: 0.84900 factor:1 | 1 (-0.99474) | -1 | -1 |
| G: -5312.08863 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.46435 HOMO: -6.60148 LUMO: -0.78369 factor:1 | 1 (-1.01003) | -1 | -1 |
| G: -5312.08863 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.85116 HOMO: -6.86543 LUMO: -0.93063 factor:1 | 1 (-1.39684) | -1 | -1 |
| G: -5312.08863 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11578.06088 HOMO: -6.70489 LUMO: -0.72382 factor:1 | 1 (-1.60656) | -1 | -1 |
| G: -5312.08863 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11578.02202 HOMO: -6.59060 LUMO: 0.31293 factor:1 | 1 (-1.56770) | -1 | -1 |
| G: -5312.08863 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11578.21381 HOMO: -6.52257 LUMO: -0.48708 factor:1 | 1 (-1.75949) | -1 | -1 |
| G: -5312.08863 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.77380 HOMO: -6.54706 LUMO: -0.48164 factor:1 | 1 (-1.31948) | -1 | -1 |
| G: -5312.08863 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11578.00850 HOMO: -7.32803 LUMO: 0.08436 factor:1 | 1 (-1.55418) | -1 | -1 |
| G: -5312.08863 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.95089 HOMO: -6.77291 LUMO: -0.66940 factor:1 | 1 (-1.49657) | -1 | -1 |
| G: -5312.08863 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11578.06075 HOMO: -6.68312 LUMO: -0.53062 factor:1 | 1 (-1.60642) | -1 | -1 |
| G: -5312.08863 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.89399 HOMO: -7.07768 LUMO: 0.45987 factor:1 | 1 (-1.43967) | -1 | -1 |
| G: -5312.08863 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11578.14146 HOMO: -6.50352 LUMO: -0.63675 factor:1 | 1 (-1.68713) | -1 | -1 |
| G: -5312.08863 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.70452 HOMO: -6.48992 LUMO: -0.60681 factor:1 | 1 (-1.25020) | -1 | -1 |
| G: -5312.08863 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.86997 HOMO: -6.65318 LUMO: -0.72382 factor:1 | 1 (-1.41565) | -1 | -1 |
| G: -5312.08863 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.77571 HOMO: -6.54706 LUMO: 0.24218 factor:1 | 1 (-1.32138) | -1 | -1 |
| G: -5312.08863 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.81361 HOMO: -6.63958 LUMO: 0.57416 factor:1 | 1 (-1.35929) | -1 | -1 |
| G: -5312.08863 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.86338 HOMO: -6.37563 LUMO: -0.48164 factor:1 | 1 (-1.40906) | -1 | -1 |
| G: -5312.08863 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11578.22701 HOMO: -6.64774 LUMO: -0.71838 factor:1 | 1 (-1.77269) | -1 | -1 |
| G: -5312.08863 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11578.04143 HOMO: -7.17020 LUMO: 0.45987 factor:1 | 1 (-1.58710) | -1 | -1 |
| G: -5312.08863 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11578.00494 HOMO: -6.86543 LUMO: -1.05036 factor:1 | 1 (-1.55061) | -1 | -1 |
| G: -5312.08863 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.23273 HOMO: -6.77019 LUMO: -1.03131 factor:1 | 1 (-0.77841) | -1 | -1 |
| G: -5312.08863 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.31940 HOMO: -6.80285 LUMO: 1.05852 factor:1 | 1 (-0.86508) | -1 | -1 |
| G: -5312.08863 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.90151 HOMO: -6.76475 LUMO: 1.01771 factor:1 | 1 (-0.44719) | -1 | -1 |
| G: -5312.08863 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.00786 HOMO: -6.92530 LUMO: 1.37417 factor:1 | 1 (-0.55353) | -1 | -1 |
| G: -5312.08863 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.24511 HOMO: -6.98244 LUMO: 1.25989 factor:1 | 1 (-0.79079) | -1 | -1 |
| G: -5312.08863 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.43682 HOMO: -6.74842 LUMO: 0.89798 factor:1 | 1 (-0.98249) | -1 | -1 |
| G: -5312.08863 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.83966 HOMO: -6.77019 LUMO: -1.17009 factor:1 | 1 (-0.38534) | -1 | -1 |
| G: -5312.08863 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.07820 HOMO: -6.78652 LUMO: 1.35785 factor:1 | 1 (-0.62388) | -1 | -1 |
| G: -5312.08863 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.27589 HOMO: -6.82734 LUMO: -0.68301 factor:1 | 1 (-0.82157) | -1 | -1 |
| G: -5312.08863 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.84099 HOMO: -6.48175 LUMO: -2.19052 factor:1 | 1 (-1.38667) | -1 | -1 |
| G: -5312.08863 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.84602 HOMO: -6.65863 LUMO: -0.77008 factor:1 | 1 (-1.39170) | -1 | -1 |
| G: -5312.08863 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.77715 HOMO: -6.44094 LUMO: -2.20956 factor:1 | 1 (-1.32283) | -1 | -1 |
| G: -5312.08863 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.77601 HOMO: -6.59876 LUMO: -0.57688 factor:1 | 1 (-1.32168) | -1 | -1 |
| G: -5312.08863 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.84099 HOMO: -6.78380 LUMO: -0.77008 factor:1 | 1 (-1.38667) | -1 | -1 |
| G: -5312.08863 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.76071 HOMO: -7.30354 LUMO: 0.25034 factor:1 | 1 (-1.30639) | -1 | -1 |
| G: -5312.08863 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.82929 HOMO: -6.59332 LUMO: -0.53334 factor:1 | 1 (-1.37496) | -1 | -1 |
| G: -5312.08863 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.83998 HOMO: -6.64230 LUMO: -0.55783 factor:1 | 1 (-1.38566) | -1 | -1 |
| G: -5312.08863 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11578.06382 HOMO: -7.26544 LUMO: 0.20409 factor:1 | 1 (-1.60950) | -1 | -1 |
| G: -5312.08863 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11578.05656 HOMO: -6.61237 LUMO: -0.65307 factor:1 | 1 (-1.60223) | -1 | -1 |
| G: -5312.08863 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.78877 HOMO: -6.72393 LUMO: -0.65307 factor:1 | 1 (-1.33445) | -1 | -1 |
| G: -5312.08863 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.94172 HOMO: -6.29671 LUMO: -0.39729 factor:1 | 1 (-1.48740) | -1 | -1 |
| G: -5312.08863 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.96847 HOMO: -6.75387 LUMO: -0.53334 factor:1 | 1 (-1.51415) | -1 | -1 |
| G: -5312.08863 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.95070 HOMO: -6.53073 LUMO: -0.31293 factor:1 | 1 (-1.49638) | -1 | -1 |
| G: -5312.08863 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.86142 HOMO: -6.42189 LUMO: -0.59049 factor:1 | 1 (-1.40710) | -1 | -1 |
| G: -5312.08863 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.97636 HOMO: -6.41100 LUMO: -0.29933 factor:1 | 1 (-1.52204) | -1 | -1 |
| G: -5312.08863 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.71573 HOMO: -6.57427 LUMO: -0.53879 factor:1 | 1 (-1.26141) | -1 | -1 |
| G: -5312.08863 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11578.05544 HOMO: -7.43143 LUMO: 0.33470 factor:1 | 1 (-1.60112) | -1 | -1 |
| G: -5312.08863 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11578.06317 HOMO: -6.56067 LUMO: -0.50885 factor:1 | 1 (-1.60885) | -1 | -1 |
| G: -5312.08863 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11578.09218 HOMO: -6.65863 LUMO: -0.76464 factor:1 | 1 (-1.63785) | -1 | -1 |
| G: -5312.08863 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.77130 HOMO: -6.32665 LUMO: -0.41906 factor:1 | 1 (-1.31698) | -1 | -1 |
| G: -5312.08863 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.76115 HOMO: -6.57699 LUMO: 1.63813 factor:1 | 1 (-1.30683) | -1 | -1 |
| G: -5312.08863 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11578.03054 HOMO: -6.53073 LUMO: 1.71704 factor:1 | 1 (-1.57622) | -1 | -1 |
| G: -5312.08863 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.76855 HOMO: -6.86271 LUMO: 2.07351 factor:1 | 1 (-1.31423) | -1 | -1 |
| G: -5312.08863 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.89979 HOMO: -6.63686 LUMO: 1.78235 factor:1 | 1 (-1.44547) | -1 | -1 |
| G: -5312.08863 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.75244 HOMO: -6.60965 LUMO: 1.94289 factor:1 | 1 (-1.29812) | -1 | -1 |
| G: -5312.08863 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.68357 HOMO: -6.55250 LUMO: 1.89119 factor:1 | 1 (-1.22925) | -1 | -1 |
| G: -5312.08863 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.96059 HOMO: -6.50624 LUMO: 1.85582 factor:1 | 1 (-0.50627) | -1 | -1 |
| G: -5312.08863 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.28223 HOMO: -6.06814 LUMO: 1.94561 factor:1 | 1 (-0.82791) | -1 | -1 |
| G: -5312.08863 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.07545 HOMO: -6.58788 LUMO: 2.01908 factor:1 | 1 (-0.62113) | -1 | -1 |
| G: -5312.08863 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.03052 HOMO: -6.74026 LUMO: 0.31293 factor:1 | 1 (-0.57620) | -1 | -1 |
| G: -5312.08863 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.86180 HOMO: -6.54434 LUMO: -0.42994 factor:1 | 1 (-1.40748) | -1 | -1 |
| G: -5312.08863 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.72137 HOMO: -6.94707 LUMO: 0.42994 factor:1 | 1 (-1.26704) | -1 | -1 |
| G: -5312.08863 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11578.10442 HOMO: -6.98516 LUMO: 0.41361 factor:1 | 1 (-1.65010) | -1 | -1 |
| G: -5312.08863 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.94834 HOMO: -6.31304 LUMO: -0.54967 factor:1 | 1 (-1.49401) | -1 | -1 |
| G: -5312.08863 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.93908 HOMO: -6.48447 LUMO: -0.40817 factor:1 | 1 (-1.48476) | -1 | -1 |
| G: -5312.08863 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11578.05239 HOMO: -6.49264 LUMO: 0.29116 factor:1 | 1 (-1.59807) | -1 | -1 |
| G: -5312.08863 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.78537 HOMO: -6.48719 LUMO: -0.11973 factor:1 | 1 (-1.33104) | -1 | -1 |
| G: -5312.08863 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.85157 HOMO: -7.16204 LUMO: 0.44082 factor:1 | 1 (-1.39725) | -1 | -1 |
| G: -5312.08863 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11578.03854 HOMO: -6.74842 LUMO: -0.37552 factor:1 | 1 (-1.58422) | -1 | -1 |
| G: -5312.08863 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11578.06763 HOMO: -6.44638 LUMO: -0.45171 factor:1 | 1 (-1.61331) | -1 | -1 |
| G: -5312.08863 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11578.09294 HOMO: -7.07496 LUMO: 0.50341 factor:1 | 1 (-1.63862) | -1 | -1 |
| G: -5312.08863 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.93631 HOMO: -6.79468 LUMO: 0.11429 factor:1 | 1 (-1.48199) | -1 | -1 |
| G: -5312.08863 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.77212 HOMO: -6.63958 LUMO: -0.67484 factor:1 | 1 (-1.31779) | -1 | -1 |
| G: -5312.08863 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.61630 HOMO: -7.08584 LUMO: 0.46259 factor:1 | 1 (-1.16198) | -1 | -1 |
| G: -5312.08863 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.80455 HOMO: -6.80285 LUMO: -0.73199 factor:1 | 1 (-1.35023) | -1 | -1 |
| G: -5312.08863 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.87865 HOMO: -6.44366 LUMO: -0.45443 factor:1 | 1 (-1.42433) | -1 | -1 |
| G: -5312.08863 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.74014 HOMO: -6.75931 LUMO: 0.25851 factor:1 | 1 (-1.28582) | -1 | -1 |
| G: -5312.08863 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.56972 HOMO: -6.64502 LUMO: 1.79323 factor:1 | 1 (-1.11539) | -1 | -1 |
| G: -5312.08863 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.44552 HOMO: -6.51168 LUMO: 1.60275 factor:1 | 1 (-0.99120) | -1 | -1 |
| G: -5312.08863 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.59935 HOMO: -6.56067 LUMO: 1.63268 factor:1 | 1 (-1.14503) | -1 | -1 |
| G: -5312.08863 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.52329 HOMO: -6.56883 LUMO: 1.70615 factor:1 | 1 (-1.06897) | -1 | -1 |
| G: -5312.08863 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.71383 HOMO: -6.77836 LUMO: 1.77962 factor:1 | 1 (-1.25951) | -1 | -1 |
| G: -5312.08863 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.42596 HOMO: -6.38923 LUMO: 1.85854 factor:1 | 1 (-0.97164) | -1 | -1 |
| G: -5312.08863 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.65685 HOMO: -6.35658 LUMO: 2.16875 factor:1 | 1 (-1.20253) | -1 | -1 |
| G: -5312.08863 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.50610 HOMO: -6.83006 LUMO: 2.31025 factor:1 | 1 (-1.05177) | -1 | -1 |
| G: -5312.08863 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.60893 HOMO: -6.87087 LUMO: 1.79051 factor:1 | 1 (-1.15461) | -1 | -1 |
| G: -5312.08863 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.82452 HOMO: -6.56339 LUMO: 2.37828 factor:1 | 1 (-1.37020) | -1 | -1 |
| G: -5312.08863 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.53584 HOMO: -6.30488 LUMO: 2.51705 factor:1 | 1 (-1.08152) | -1 | -1 |
| G: -5312.08863 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.48803 HOMO: -6.69400 LUMO: 1.95650 factor:1 | 1 (-1.03371) | -1 | -1 |
| G: -5312.08863 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.43894 HOMO: -6.51168 LUMO: 2.03541 factor:1 | 1 (-0.98462) | -1 | -1 |
| G: -5312.08863 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.72343 HOMO: -6.30760 LUMO: 1.65173 factor:1 | 1 (-1.26911) | -1 | -1 |
| G: -5312.08863 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.63081 HOMO: -6.55250 LUMO: 1.90752 factor:1 | 1 (-1.17648) | -1 | -1 |
| G: -5312.08863 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.70928 HOMO: -6.41372 LUMO: 1.76058 factor:1 | 1 (-1.25496) | -1 | -1 |
| G: -5312.08863 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.74349 HOMO: -6.23957 LUMO: 2.06534 factor:1 | 1 (-1.28917) | -1 | -1 |
| G: -5312.08863 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.83481 HOMO: -6.58243 LUMO: 2.11705 factor:1 | 1 (-1.38049) | -1 | -1 |
| G: -5312.08863 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11578.05411 HOMO: -6.37835 LUMO: 2.09256 factor:1 | 1 (-1.59978) | -1 | -1 |
| G: -5312.08863 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.79761 HOMO: -6.50624 LUMO: 2.55787 factor:1 | 1 (-1.34329) | -1 | -1 |
| G: -5312.08863 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.76428 HOMO: -6.45454 LUMO: 1.87214 factor:1 | 1 (-1.30996) | -1 | -1 |
| G: -5312.08863 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.75108 HOMO: -6.53617 LUMO: 1.95650 factor:1 | 1 (-1.29676) | -1 | -1 |
| G: -5312.08863 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.91136 HOMO: -6.51985 LUMO: 1.71432 factor:1 | 1 (-1.45703) | -1 | -1 |
| G: -5312.08863 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.70488 HOMO: -6.75114 LUMO: 1.84493 factor:1 | 1 (-1.25055) | -1 | -1 |
| G: -5312.08863 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.78934 HOMO: -6.06270 LUMO: 1.65717 factor:1 | 1 (-1.33502) | -1 | -1 |
| G: -5312.08863 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.48343 HOMO: -5.89671 LUMO: 1.71704 factor:1 | 1 (-1.02911) | -1 | -1 |
| G: -5312.08863 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.43818 HOMO: -6.18787 LUMO: 1.91840 factor:1 | 1 (-0.98385) | -1 | -1 |
| G: -5312.08863 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.54229 HOMO: -6.01644 LUMO: 1.85582 factor:1 | 1 (-1.08797) | -1 | -1 |
| G: -5312.08863 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.43543 HOMO: -6.05998 LUMO: 2.33474 factor:1 | 1 (-0.98111) | -1 | -1 |
| G: -5312.08863 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.34990 HOMO: -6.05725 LUMO: 2.03541 factor:1 | 1 (-0.89558) | -1 | -1 |
| G: -5312.08863 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.39061 HOMO: -6.80829 LUMO: 1.90480 factor:1 | 1 (-0.93629) | -1 | -1 |
| G: -5312.08863 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.64136 HOMO: -6.76475 LUMO: 2.20956 factor:1 | 1 (-1.18704) | -1 | -1 |
| G: -5312.08863 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.42732 HOMO: -6.29944 LUMO: 1.77962 factor:1 | 1 (-0.97300) | -1 | -1 |
| G: -5312.08863 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.73405 HOMO: -6.47359 LUMO: -0.25579 factor:1 | 1 (-1.27972) | -1 | -1 |
| G: -5312.08863 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.48950 HOMO: -6.57699 LUMO: -0.47348 factor:1 | 1 (-1.03518) | -1 | -1 |
| G: -5312.08863 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.33015 HOMO: -7.20830 LUMO: 0.49797 factor:1 | 1 (-0.87583) | -1 | -1 |
| G: -5312.08863 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.27763 HOMO: -7.49402 LUMO: 0.29933 factor:1 | 1 (-0.82331) | -1 | -1 |
| G: -5312.08863 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.17774 HOMO: -6.66679 LUMO: -0.58777 factor:1 | 1 (-0.72341) | -1 | -1 |
| G: -5312.08863 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.93550 HOMO: -6.67767 LUMO: -0.56328 factor:1 | 1 (-0.48118) | -1 | -1 |
| G: -5312.08863 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.42231 HOMO: -7.42871 LUMO: 0.35647 factor:1 | 1 (-0.96799) | -1 | -1 |
| G: -5312.08863 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.22381 HOMO: -6.56067 LUMO: -0.54423 factor:1 | 1 (-0.76948) | -1 | -1 |
| G: -5312.08863 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.11708 HOMO: -6.56339 LUMO: -0.50341 factor:1 | 1 (-0.66276) | -1 | -1 |
| G: -5312.08863 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.60969 HOMO: -6.56067 LUMO: -0.48436 factor:1 | 1 (-1.15537) | -1 | -1 |
| G: -5312.08863 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.16239 HOMO: -6.73210 LUMO: 1.75241 factor:1 | 1 (-0.70807) | -1 | -1 |
| G: -5312.08863 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.27962 HOMO: -6.48175 LUMO: 1.91296 factor:1 | 1 (-0.82529) | -1 | -1 |
| G: -5312.08863 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.36359 HOMO: -6.67767 LUMO: 1.70343 factor:1 | 1 (-0.90927) | -1 | -1 |
| G: -5312.08863 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11578.11743 HOMO: -6.37835 LUMO: 1.96466 factor:1 | 1 (-1.66311) | -1 | -1 |
| G: -5312.08863 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11578.01816 HOMO: -6.40828 LUMO: 2.10072 factor:1 | 1 (-1.56384) | -1 | -1 |
| G: -5312.08863 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11578.34641 HOMO: -6.06542 LUMO: 1.92112 factor:1 | 1 (-1.89209) | -1 | -1 |
| G: -5312.08863 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.81614 HOMO: -6.90353 LUMO: 1.83133 factor:1 | 1 (-1.36182) | -1 | -1 |
| G: -5312.08863 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11578.72579 HOMO: -6.37019 LUMO: 1.92929 factor:1 | 1 (-2.27147) | -1 | -1 |
| G: -5312.08863 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11578.20976 HOMO: -6.61509 LUMO: 2.11160 factor:1 | 1 (-1.75543) | -1 | -1 |
| G: -5312.08863 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11578.40336 HOMO: -6.82734 LUMO: 1.77146 factor:1 | 1 (-1.94904) | -1 | -1 |
| G: -5312.08863 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11578.39887 HOMO: -6.01100 LUMO: 1.89935 factor:1 | 1 (-1.94455) | -1 | -1 |
| G: -5312.08863 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11578.77831 HOMO: -6.49536 LUMO: 1.75241 factor:1 | 1 (-2.32399) | -1 | -1 |
| G: -5312.08863 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11578.21773 HOMO: -6.34297 LUMO: 1.86398 factor:1 | 1 (-1.76341) | -1 | -1 |
| G: -5312.08863 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11578.53074 HOMO: -6.53073 LUMO: 1.84493 factor:1 | 1 (-2.07642) | -1 | -1 |
| G: -5312.08863 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11579.08836 HOMO: -6.53345 LUMO: 2.41093 factor:1 | 1 (-2.63403) | -1 | -1 |
| G: -5312.08863 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11578.82120 HOMO: -7.01237 LUMO: 2.06262 factor:1 | 1 (-2.36687) | -1 | -1 |
| G: -5312.08863 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11578.27542 HOMO: -6.17154 LUMO: 1.89119 factor:1 | 1 (-1.82109) | -1 | -1 |
| G: -5312.08863 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11578.38184 HOMO: -6.08719 LUMO: 1.74425 factor:1 | 1 (-1.92752) | -1 | -1 |
| G: -5312.08863 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11578.16682 HOMO: -6.69672 LUMO: 1.95106 factor:1 | 1 (-1.71249) | -1 | -1 |
| G: -5312.08863 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11579.02120 HOMO: -6.58243 LUMO: 2.24766 factor:1 | 1 (-2.56688) | -1 | -1 |
| G: -5312.08863 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11578.83913 HOMO: -6.74570 LUMO: 2.02181 factor:1 | 1 (-2.38481) | -1 | -1 |
| G: -5312.08863 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11578.03351 HOMO: -6.53890 LUMO: 1.92929 factor:1 | 1 (-1.57919) | -1 | -1 |
| G: -5312.08863 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11578.23299 HOMO: -6.03276 LUMO: 1.67078 factor:1 | 1 (-1.77867) | -1 | -1 |
| G: -5312.08863 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.84477 HOMO: -6.67767 LUMO: 2.03541 factor:1 | 1 (-1.39045) | -1 | -1 |
| G: -5312.08863 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.79947 HOMO: -5.98378 LUMO: 1.84221 factor:1 | 1 (-0.34515) | -1 | -1 |
| G: -5312.08863 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.84769 HOMO: -6.07086 LUMO: 2.01908 factor:1 | 1 (-0.39337) | -1 | -1 |
| G: -5312.08863 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.86249 HOMO: -6.29944 LUMO: 1.90208 factor:1 | 1 (-0.40817) | -1 | -1 |
| G: -5312.08863 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.62652 HOMO: -6.75114 LUMO: 1.85854 factor:1 | 1 (-0.17219) | -1 | -1 |
| G: -5312.08863 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.73604 HOMO: -6.56611 LUMO: 2.49801 factor:1 | 1 (-0.28172) | -1 | -1 |
| G: -5312.08863 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.66398 HOMO: -6.39740 LUMO: 1.92929 factor:1 | 1 (-1.20965) | -1 | -1 |
| G: -5312.08863 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.89965 HOMO: -6.85999 LUMO: -1.07757 factor:1 | 1 (-1.44533) | -1 | -1 |
| G: -5312.08863 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.91835 HOMO: -6.98244 LUMO: 1.07213 factor:1 | 1 (-1.46403) | -1 | -1 |
| G: -5312.08863 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.59715 HOMO: -7.04231 LUMO: 0.64219 factor:1 | 1 (-1.14282) | -1 | -1 |
| G: -5312.08863 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.86385 HOMO: -6.96339 LUMO: 0.75648 factor:1 | 1 (-0.40953) | -1 | -1 |
| G: -5312.08863 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.86021 HOMO: -6.83822 LUMO: -0.97417 factor:1 | 1 (-0.40589) | -1 | -1 |
| G: -5312.08863 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.02035 HOMO: -6.44910 LUMO: -2.15242 factor:1 | 1 (-0.56602) | -1 | -1 |
| G: -5312.08863 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.22378 HOMO: -6.84094 LUMO: -1.37690 factor:1 | 1 (-0.76946) | -1 | -1 |
| G: -5312.08863 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.09305 HOMO: -6.74026 LUMO: -2.54699 factor:1 | 1 (-0.63873) | -1 | -1 |
| G: -5312.08863 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.71770 HOMO: -6.96611 LUMO: 1.24900 factor:1 | 1 (-0.26338) | -1 | -1 |
| G: -5312.08863 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.80674 HOMO: -7.21102 LUMO: 0.82995 factor:1 | 1 (-0.35241) | -1 | -1 |
| G: -5312.08863 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.72845 HOMO: -6.88448 LUMO: 0.81634 factor:1 | 1 (-0.27413) | -1 | -1 |
| G: -5312.08863 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.05586 HOMO: -7.04231 LUMO: 1.10750 factor:1 | 1 (-0.60153) | -1 | -1 |
| G: -5312.08863 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.82402 HOMO: -6.83550 LUMO: -0.98777 factor:1 | 1 (-0.36969) | -1 | -1 |
| G: -5312.08863 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.98347 HOMO: -6.82189 LUMO: 0.93879 factor:1 | 1 (-0.52915) | -1 | -1 |
| G: -5312.08863 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.21616 HOMO: -6.81101 LUMO: 0.70750 factor:1 | 1 (-0.76184) | -1 | -1 |
| G: -5312.08863 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.55585 HOMO: -7.06680 LUMO: 0.74015 factor:1 | 1 (-0.10153) | -1 | -1 |
| G: -5312.08863 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.69454 HOMO: -6.68856 LUMO: 0.86260 factor:1 | 1 (-0.24022) | -1 | -1 |
| G: -5312.08863 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.89047 HOMO: -6.83822 LUMO: -0.63403 factor:1 | 1 (-0.43614) | -1 | -1 |
| G: -5312.08863 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.68799 HOMO: -6.84911 LUMO: 1.26533 factor:1 | 1 (-0.23366) | -1 | -1 |
| G: -5312.08863 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.13257 HOMO: -7.01237 LUMO: 0.73743 factor:1 | 1 (-0.67824) | -1 | -1 |
| G: -5312.08863 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.19061 HOMO: -7.00965 LUMO: 1.40139 factor:1 | 1 (-0.73629) | -1 | -1 |
| G: -5312.08863 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.92418 HOMO: -6.73210 LUMO: -2.49256 factor:1 | 1 (-0.46986) | -1 | -1 |
| G: -5312.08863 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.76323 HOMO: -7.08040 LUMO: 0.84627 factor:1 | 1 (-0.30890) | -1 | -1 |
| G: -5312.08863 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.61057 HOMO: -7.00965 LUMO: 0.82995 factor:1 | 1 (-0.15625) | -1 | -1 |
| G: -5312.08863 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11578.08398 HOMO: -6.88448 LUMO: 0.82723 factor:1 | 1 (-1.62966) | -1 | -1 |
| G: -5312.08863 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11579.01891 HOMO: -7.20013 LUMO: 0.88437 factor:1 | 1 (-2.56459) | -1 | -1 |
| G: -5312.08863 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11578.31131 HOMO: -6.60420 LUMO: -0.53334 factor:1 | 1 (-1.85699) | -1 | -1 |
| G: -5312.08863 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11578.02292 HOMO: -6.78652 LUMO: -0.79729 factor:1 | 1 (-1.56860) | -1 | -1 |
| G: -5312.08863 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.78320 HOMO: -6.48992 LUMO: -0.64491 factor:1 | 1 (-0.32888) | -1 | -1 |
| G: -5312.08863 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.75087 HOMO: -6.85999 LUMO: -0.78097 factor:1 | 1 (-0.29655) | -1 | -1 |
| G: -5312.08863 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.07145 HOMO: -6.65046 LUMO: -0.78097 factor:1 | 1 (-0.61713) | -1 | -1 |
| G: -5312.08863 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.99123 HOMO: -7.24095 LUMO: 0.37280 factor:1 | 1 (-0.53691) | -1 | -1 |
| G: -5312.08863 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.66284 HOMO: -6.81101 LUMO: -0.74831 factor:1 | 1 (-0.20852) | -1 | -1 |
| G: -5312.08863 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.77301 HOMO: -6.69400 LUMO: -0.77280 factor:1 | 1 (-1.31869) | -1 | -1 |
| G: -5312.08863 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11578.40494 HOMO: -6.08447 LUMO: -0.68573 factor:1 | 1 (-1.95062) | -1 | -1 |
| G: -5312.08863 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.74382 HOMO: -6.66679 LUMO: -0.47076 factor:1 | 1 (-1.28949) | -1 | -1 |
| G: -5312.08863 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.99171 HOMO: -6.97428 LUMO: -1.10750 factor:1 | 1 (-1.53739) | -1 | -1 |
| G: -5312.08863 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.68654 HOMO: -6.69128 LUMO: -0.54151 factor:1 | 1 (-1.23221) | -1 | -1 |
| G: -5312.08863 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.69530 HOMO: -6.53617 LUMO: -0.35375 factor:1 | 1 (-1.24098) | -1 | -1 |
| G: -5312.08863 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.91348 HOMO: -6.75659 LUMO: -0.41361 factor:1 | 1 (-1.45916) | -1 | -1 |
| G: -5312.08863 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.92741 HOMO: -6.69400 LUMO: -0.67484 factor:1 | 1 (-1.47309) | -1 | -1 |
| G: -5312.08863 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.50670 HOMO: -6.89264 LUMO: -0.90886 factor:1 | 1 (-1.05237) | -1 | -1 |
| G: -5312.08863 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11578.06241 HOMO: -6.56339 LUMO: -0.52518 factor:1 | 1 (-1.60808) | -1 | -1 |
| G: -5312.08863 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.97402 HOMO: -6.45726 LUMO: -0.65852 factor:1 | 1 (-1.51970) | -1 | -1 |
| G: -5312.08863 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11578.26331 HOMO: -6.80557 LUMO: -0.56600 factor:1 | 1 (-1.80899) | -1 | -1 |
| G: -5312.08863 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.73931 HOMO: -7.19469 LUMO: -0.91702 factor:1 | 1 (-0.28498) | -1 | -1 |
| G: -5312.08863 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.83144 HOMO: -6.41100 LUMO: 0.79185 factor:1 | 1 (-0.37712) | -1 | -1 |
| G: -5312.08863 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.57781 HOMO: -6.39195 LUMO: 0.26123 factor:1 | 1 (-0.12349) | -1 | -1 |
| G: -5312.08863 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.89564 HOMO: -6.78924 LUMO: 0.35919 factor:1 | 1 (-0.44131) | -1 | -1 |
| G: -5312.08863 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.04369 HOMO: -6.50624 LUMO: 0.71838 factor:1 | 1 (-0.58937) | -1 | -1 |
| G: -5312.08863 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.61098 HOMO: -6.68584 LUMO: -0.66124 factor:1 | 1 (-0.15666) | -1 | -1 |
| G: -5312.08863 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11578.45460 HOMO: -6.45182 LUMO: -0.48980 factor:1 | 1 (-2.00028) | -1 | -1 |
| G: -5312.08863 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.63078 HOMO: -7.18925 LUMO: -1.01498 factor:1 | 1 (-1.17646) | -1 | -1 |
| G: -5312.08863 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.76730 HOMO: -7.18925 LUMO: -0.63130 factor:1 | 1 (-1.31298) | -1 | -1 |
| G: -5312.08863 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.91810 HOMO: -6.66679 LUMO: -0.57960 factor:1 | 1 (-1.46378) | -1 | -1 |
| G: -5312.08863 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11578.14880 HOMO: -6.44910 LUMO: -0.30205 factor:1 | 1 (-1.69448) | -1 | -1 |
| G: -5312.08863 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11578.33079 HOMO: -7.23279 LUMO: 0.46804 factor:1 | 1 (-1.87647) | -1 | -1 |
| G: -5312.08863 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11578.37721 HOMO: -6.92802 LUMO: -0.72927 factor:1 | 1 (-1.92289) | -1 | -1 |
| G: -5312.08863 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.91239 HOMO: -6.83278 LUMO: -0.59321 factor:1 | 1 (-1.45807) | -1 | -1 |
| G: -5312.08863 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.64634 HOMO: -7.44776 LUMO: 0.27211 factor:1 | 1 (-1.19202) | -1 | -1 |
| G: -5312.08863 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.88866 HOMO: -6.80829 LUMO: -0.59865 factor:1 | 1 (-1.43434) | -1 | -1 |
| G: -5312.08863 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.93949 HOMO: -6.63686 LUMO: -0.75103 factor:1 | 1 (-1.48517) | -1 | -1 |
| G: -5312.08863 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.66830 HOMO: -6.73210 LUMO: -0.55511 factor:1 | 1 (-1.21398) | -1 | -1 |
| G: -5312.08863 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11578.10924 HOMO: -6.50624 LUMO: 1.58642 factor:1 | 1 (-1.65491) | -1 | -1 |
| G: -5312.08863 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11578.33316 HOMO: -6.79196 LUMO: 0.96328 factor:1 | 1 (-1.87884) | -1 | -1 |
| G: -5312.08863 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11578.24845 HOMO: -6.82734 LUMO: 1.23540 factor:1 | 1 (-1.79413) | -1 | -1 |
| G: -5312.08863 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11578.01057 HOMO: -6.90081 LUMO: 1.25444 factor:1 | 1 (-1.55625) | -1 | -1 |
| G: -5312.08863 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.89724 HOMO: -7.00965 LUMO: -1.05036 factor:1 | 1 (-0.44292) | -1 | -1 |
| G: -5312.08863 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.74214 HOMO: -7.01237 LUMO: -1.48302 factor:1 | 1 (-0.28781) | -1 | -1 |
| G: -5312.08863 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.87251 HOMO: -6.91713 LUMO: 0.93607 factor:1 | 1 (-0.41818) | -1 | -1 |
| G: -5312.08863 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.94647 HOMO: -7.02598 LUMO: 0.92247 factor:1 | 1 (-0.49215) | -1 | -1 |
| G: -5312.08863 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.93477 HOMO: -6.98516 LUMO: 1.52384 factor:1 | 1 (-0.48044) | -1 | -1 |
| G: -5312.08863 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.00935 HOMO: -6.75387 LUMO: 1.04764 factor:1 | 1 (-0.55503) | -1 | -1 |
| G: -5312.08863 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.60404 HOMO: -7.09401 LUMO: 1.19458 factor:1 | 1 (-0.14972) | -1 | -1 |
| G: -5312.08863 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.82151 HOMO: -6.88992 LUMO: -1.56193 factor:1 | 1 (-0.36719) | -1 | -1 |
| G: -5312.08863 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.69709 HOMO: -7.00149 LUMO: 0.99866 factor:1 | 1 (-1.24277) | -1 | -1 |
| G: -5312.08863 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11578.51531 HOMO: -7.13755 LUMO: 1.05308 factor:1 | 1 (-2.06099) | -1 | -1 |
| G: -5312.08863 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.89508 HOMO: -6.85183 LUMO: -1.42860 factor:1 | 1 (-1.44076) | -1 | -1 |
| G: -5312.08863 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.93759 HOMO: -6.63141 LUMO: -0.88981 factor:1 | 1 (-1.48327) | -1 | -1 |
| G: -5312.08863 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.63894 HOMO: -6.92258 LUMO: -0.82178 factor:1 | 1 (-1.18462) | -1 | -1 |
| G: -5312.08863 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.71595 HOMO: -6.55794 LUMO: -0.80818 factor:1 | 1 (-1.26163) | -1 | -1 |
| G: -5312.08863 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.60123 HOMO: -6.95251 LUMO: -0.97145 factor:1 | 1 (-1.14691) | -1 | -1 |
| G: -5312.08863 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.75565 HOMO: -7.37701 LUMO: 0.14150 factor:1 | 1 (-1.30133) | -1 | -1 |
| G: -5312.08863 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.65124 HOMO: -6.74842 LUMO: -0.68028 factor:1 | 1 (-1.19692) | -1 | -1 |
| G: -5312.08863 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.98387 HOMO: -6.65046 LUMO: -0.52518 factor:1 | 1 (-1.52955) | -1 | -1 |
| G: -5312.08863 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.89887 HOMO: -6.91441 LUMO: -1.13199 factor:1 | 1 (-0.44455) | -1 | -1 |
| G: -5312.08863 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.09417 HOMO: -7.00965 LUMO: -1.00682 factor:1 | 1 (-0.63985) | -1 | -1 |
| G: -5312.08863 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.98334 HOMO: -6.55794 LUMO: -0.54967 factor:1 | 1 (-0.52902) | -1 | -1 |
| G: -5312.08863 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.03205 HOMO: -6.71577 LUMO: -0.53879 factor:1 | 1 (-0.57772) | -1 | -1 |
| G: -5312.08863 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.01289 HOMO: -6.88992 LUMO: -0.55511 factor:1 | 1 (-0.55857) | -1 | -1 |
| G: -5312.08863 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.98630 HOMO: -6.74026 LUMO: -0.60681 factor:1 | 1 (-0.53198) | -1 | -1 |
| G: -5312.08863 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.23306 HOMO: -6.76747 LUMO: -0.50885 factor:1 | 1 (-0.77874) | -1 | -1 |
| G: -5312.08863 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.17899 HOMO: -6.87904 LUMO: -0.92519 factor:1 | 1 (-0.72467) | -1 | -1 |
| G: -5312.08863 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.77172 HOMO: -6.53073 LUMO: -0.53062 factor:1 | 1 (-0.31739) | -1 | -1 |
| G: -5312.08863 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.86576 HOMO: -6.97700 LUMO: -0.98505 factor:1 | 1 (-0.41144) | -1 | -1 |
| G: -5312.08863 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.77947 HOMO: -6.96884 LUMO: -0.79185 factor:1 | 1 (-0.32515) | -1 | -1 |
| G: -5312.08863 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.99703 HOMO: -6.60420 LUMO: -0.31021 factor:1 | 1 (-0.54270) | -1 | -1 |
| G: -5312.08863 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: -0.63947 factor:1 | 1 (-0.27312) | -1 | -1 |
| G: -5312.08863 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.03088 HOMO: -6.41917 LUMO: -0.35103 factor:1 | 1 (-0.57655) | -1 | -1 |
| G: -5312.08863 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.98870 HOMO: -6.73482 LUMO: -0.70477 factor:1 | 1 (-0.53438) | -1 | -1 |
| G: -5312.08863 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.95659 HOMO: -6.71305 LUMO: -0.85716 factor:1 | 1 (-0.50227) | -1 | -1 |
| G: -5312.08863 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.06827 HOMO: -6.70761 LUMO: -0.63403 factor:1 | 1 (-0.61394) | -1 | -1 |
| G: -5312.08863 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.91120 HOMO: -6.37563 LUMO: -0.38640 factor:1 | 1 (-0.45688) | -1 | -1 |
| G: -5312.08863 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.25461 HOMO: -6.27495 LUMO: -0.54967 factor:1 | 1 (-0.80029) | -1 | -1 |
| G: -5312.08863 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.89262 HOMO: -6.98516 LUMO: 0.38096 factor:1 | 1 (-0.43829) | -1 | -1 |
| G: -5312.08863 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.63503 HOMO: -6.47087 LUMO: -0.40001 factor:1 | 1 (-0.18071) | -1 | -1 |
| G: -5312.08863 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.90687 HOMO: -6.59876 LUMO: 0.20681 factor:1 | 1 (-0.45255) | -1 | -1 |
| G: -5312.08863 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.69424 HOMO: -6.89809 LUMO: 0.14966 factor:1 | 1 (-0.23992) | -1 | -1 |
| G: -5312.08863 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.97615 HOMO: -6.76203 LUMO: 2.11432 factor:1 | 1 (-0.52183) | -1 | -1 |
| G: -5312.08863 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.05997 HOMO: -6.58516 LUMO: 1.75786 factor:1 | 1 (-0.60564) | -1 | -1 |
| G: -5312.08863 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.75988 HOMO: -6.37835 LUMO: 1.84493 factor:1 | 1 (-0.30556) | -1 | -1 |
| G: -5312.08863 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.98138 HOMO: -6.83550 LUMO: 1.74425 factor:1 | 1 (-0.52706) | -1 | -1 |
| G: -5312.08863 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.89180 HOMO: -6.65318 LUMO: 1.79051 factor:1 | 1 (-0.43748) | -1 | -1 |
| G: -5312.08863 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.85800 HOMO: -6.68584 LUMO: 2.11160 factor:1 | 1 (-0.40368) | -1 | -1 |
| G: -5312.08863 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.76976 HOMO: -6.36202 LUMO: 1.85037 factor:1 | 1 (-0.31543) | -1 | -1 |
| G: -5312.08863 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.49481 HOMO: -6.68312 LUMO: 2.23133 factor:1 | 1 (-0.04049) | -1 | -1 |
| G: -5312.08863 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.62687 HOMO: -6.66679 LUMO: 2.14154 factor:1 | 1 (-0.17255) | -1 | -1 |
| G: -5312.08863 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.54031 HOMO: -6.50896 LUMO: 1.92657 factor:1 | 1 (-0.08599) | -1 | -1 |
| G: -5312.08863 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.89172 HOMO: -6.63686 LUMO: 2.22317 factor:1 | 1 (-0.43740) | -1 | -1 |
| G: -5312.08863 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.98587 HOMO: -6.58788 LUMO: 2.17419 factor:1 | 1 (-0.53155) | -1 | -1 |
| G: -5312.08863 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.88747 HOMO: -6.72665 LUMO: 2.12249 factor:1 | 1 (-0.43315) | -1 | -1 |
| G: -5312.08863 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.07205 HOMO: -6.28311 LUMO: 1.91024 factor:1 | 1 (-0.61773) | -1 | -1 |
| G: -5312.08863 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.73454 HOMO: -6.56067 LUMO: 2.27487 factor:1 | 1 (-0.28022) | -1 | -1 |
| G: -5312.08863 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.13338 HOMO: -6.83006 LUMO: 2.28031 factor:1 | 1 (-0.67906) | -1 | -1 |
| G: -5312.08863 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.00307 HOMO: -6.45182 LUMO: 1.62724 factor:1 | 1 (-0.54874) | -1 | -1 |
| G: -5312.08863 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.07828 HOMO: -6.78380 LUMO: 1.83677 factor:1 | 1 (-0.62396) | -1 | -1 |
| G: -5312.08863 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.34928 HOMO: -6.23413 LUMO: 1.80956 factor:1 | 1 (-0.89496) | -1 | -1 |
| G: -5312.08863 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.16389 HOMO: -6.74298 LUMO: 2.16875 factor:1 | 1 (-0.70956) | -1 | -1 |
| G: -5312.08863 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.98269 HOMO: -6.81645 LUMO: 2.50073 factor:1 | 1 (-0.52836) | -1 | -1 |
| G: -5312.08863 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.92598 HOMO: -6.71033 LUMO: 1.96466 factor:1 | 1 (-0.47165) | -1 | -1 |
| G: -5312.08863 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.99847 HOMO: -6.83550 LUMO: 2.04358 factor:1 | 1 (-0.54415) | -1 | -1 |
| G: -5312.08863 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.17564 HOMO: -6.60965 LUMO: 2.38100 factor:1 | 1 (-0.72132) | -1 | -1 |
| G: -5312.08863 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.10756 HOMO: -6.73210 LUMO: 2.26127 factor:1 | 1 (-0.65324) | -1 | -1 |
| G: -5312.08863 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.14965 HOMO: -6.76203 LUMO: 2.13609 factor:1 | 1 (-0.69533) | -1 | -1 |
| G: -5312.08863 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.28718 HOMO: -6.71033 LUMO: 2.05990 factor:1 | 1 (-0.83286) | -1 | -1 |
| G: -5312.08863 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.83634 HOMO: -6.50896 LUMO: 2.32385 factor:1 | 1 (-0.38202) | -1 | -1 |
| G: -5312.08863 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.87689 HOMO: -6.53345 LUMO: 1.74425 factor:1 | 1 (-0.42257) | -1 | -1 |
| G: -5312.08863 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.76159 HOMO: -6.25862 LUMO: 1.63540 factor:1 | 1 (-0.30727) | -1 | -1 |
| G: -5312.08863 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.96622 HOMO: -5.90759 LUMO: 1.78779 factor:1 | 1 (-0.51190) | -1 | -1 |
| G: -5312.08863 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.91131 HOMO: -6.09807 LUMO: 1.99732 factor:1 | 1 (-0.45699) | -1 | -1 |
| G: -5312.08863 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.75297 HOMO: -5.92392 LUMO: 1.99732 factor:1 | 1 (-0.29864) | -1 | -1 |
| G: -5312.08863 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.09314 HOMO: -6.45182 LUMO: 1.72248 factor:1 | 1 (-0.63881) | -1 | -1 |
| G: -5312.08863 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.01210 HOMO: -6.53073 LUMO: 1.82588 factor:1 | 1 (-0.55778) | -1 | -1 |
| G: -5312.08863 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.00995 HOMO: -6.40828 LUMO: 2.05174 factor:1 | 1 (-0.55563) | -1 | -1 |
| G: -5312.08863 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.68614 HOMO: -6.60420 LUMO: -0.82450 factor:1 | 1 (-0.23181) | -1 | -1 |
| G: -5312.08863 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.64532 HOMO: -6.76747 LUMO: -0.57144 factor:1 | 1 (-0.19100) | -1 | -1 |
| G: -5312.08863 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.46450 HOMO: -6.67767 LUMO: -0.59321 factor:1 | 1 (-0.01018) | -1 | -1 |
| G: -5312.08863 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.57027 HOMO: -6.65863 LUMO: -0.57416 factor:1 | 1 (-0.11595) | -1 | -1 |
| G: -5312.08863 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.93199 HOMO: -6.49808 LUMO: -0.54695 factor:1 | 1 (-0.47767) | -1 | -1 |
| G: -5312.08863 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.86516 HOMO: -6.50080 LUMO: -0.61498 factor:1 | 1 (-0.41084) | -1 | -1 |
| G: -5312.08863 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.87806 HOMO: -6.74842 LUMO: -0.51974 factor:1 | 1 (-0.42374) | -1 | -1 |
| G: -5312.08863 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.01920 HOMO: -6.13345 LUMO: 0.67756 factor:1 | 1 (-0.56488) | -1 | -1 |
| G: -5312.08863 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.99382 HOMO: -6.48719 LUMO: 0.52790 factor:1 | 1 (-0.53949) | -1 | -1 |
| G: -5312.08863 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.21148 HOMO: -6.35930 LUMO: 0.74015 factor:1 | 1 (-0.75716) | -1 | -1 |
| G: -5312.08863 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.05012 HOMO: -6.41644 LUMO: 0.22313 factor:1 | 1 (-0.59579) | -1 | -1 |
| G: -5312.08863 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.05969 HOMO: -6.85727 LUMO: -0.00272 factor:1 | 1 (-0.60537) | -1 | -1 |
| G: -5312.08863 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.91713 HOMO: -6.84638 LUMO: 0.24762 factor:1 | 1 (-0.46281) | -1 | -1 |
| G: -5312.08863 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.74649 HOMO: -6.66951 LUMO: 0.39184 factor:1 | 1 (-0.29217) | -1 | -1 |
| G: -5312.08863 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.71291 HOMO: -6.62597 LUMO: -0.65035 factor:1 | 1 (-0.25859) | -1 | -1 |
| G: -5312.08863 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.62253 HOMO: -7.13755 LUMO: 0.45715 factor:1 | 1 (-1.16821) | -1 | -1 |
| G: -5312.08863 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.46533 HOMO: -7.12666 LUMO: 0.45171 factor:1 | 1 (-1.01101) | -1 | -1 |
| G: -5312.08863 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.58476 HOMO: -6.46270 LUMO: -0.46259 factor:1 | 1 (-1.13044) | -1 | -1 |
| G: -5312.08863 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.75299 HOMO: -6.36202 LUMO: -0.29660 factor:1 | 1 (-1.29866) | -1 | -1 |
| G: -5312.08863 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.85318 HOMO: -6.28583 LUMO: 0.40545 factor:1 | 1 (-1.39886) | -1 | -1 |
| G: -5312.08863 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.64346 HOMO: -6.70761 LUMO: 0.41906 factor:1 | 1 (-1.18914) | -1 | -1 |
| G: -5312.08863 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.48506 HOMO: -6.76203 LUMO: -0.60954 factor:1 | 1 (-1.03074) | -1 | -1 |
| G: -5312.08863 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.33309 HOMO: -6.85999 LUMO: -0.75103 factor:1 | 1 (-0.87876) | -1 | -1 |
| G: -5312.08863 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.73184 HOMO: -7.19741 LUMO: -1.00954 factor:1 | 1 (-1.27752) | -1 | -1 |
| G: -5312.08863 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11578.19977 HOMO: -6.58243 LUMO: -0.33470 factor:1 | 1 (-1.74545) | -1 | -1 |
| G: -5312.08863 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11578.08622 HOMO: -7.22190 LUMO: 0.49253 factor:1 | 1 (-1.63189) | -1 | -1 |
| G: -5312.08863 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11578.23781 HOMO: -7.22462 LUMO: 0.51974 factor:1 | 1 (-1.78349) | -1 | -1 |
| G: -5312.08863 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11578.80296 HOMO: -7.08584 LUMO: -0.68301 factor:1 | 1 (-2.34864) | -1 | -1 |
| G: -5312.08863 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11579.10817 HOMO: -6.68584 LUMO: -0.29660 factor:1 | 1 (-2.65384) | -1 | -1 |
| G: -5312.08863 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11578.32276 HOMO: -6.33753 LUMO: -0.48436 factor:1 | 1 (-1.86844) | -1 | -1 |
| G: -5312.08863 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.77533 HOMO: -7.15932 LUMO: 0.55511 factor:1 | 1 (-1.32100) | -1 | -1 |
| G: -5312.08863 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.98591 HOMO: -6.57427 LUMO: 2.01908 factor:1 | 1 (-1.53159) | -1 | -1 |
| G: -5312.08863 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.87840 HOMO: -6.75659 LUMO: 2.22045 factor:1 | 1 (-1.42408) | -1 | -1 |
| G: -5312.08863 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.97277 HOMO: -6.73482 LUMO: 2.20956 factor:1 | 1 (-1.51845) | -1 | -1 |
| G: -5312.08863 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.69840 HOMO: -6.74026 LUMO: 1.76602 factor:1 | 1 (-1.24408) | -1 | -1 |
| G: -5312.08863 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.94856 HOMO: -6.95523 LUMO: 1.94834 factor:1 | 1 (-0.49424) | -1 | -1 |
| G: -5312.08863 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.87166 HOMO: -6.33209 LUMO: 1.87486 factor:1 | 1 (-0.41734) | -1 | -1 |
| G: -5312.08863 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.90965 HOMO: -6.71033 LUMO: 2.12521 factor:1 | 1 (-0.45533) | -1 | -1 |
| G: -5312.08863 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.00655 HOMO: -6.50080 LUMO: 2.04902 factor:1 | 1 (-0.55223) | -1 | -1 |
| G: -5312.08863 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.11714 HOMO: -6.76475 LUMO: 1.94017 factor:1 | 1 (-0.66281) | -1 | -1 |
| G: -5312.08863 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.12220 HOMO: -6.53073 LUMO: 2.08983 factor:1 | 1 (-0.66788) | -1 | -1 |
| G: -5312.08863 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.85648 HOMO: -6.69944 LUMO: 2.20684 factor:1 | 1 (-0.40216) | -1 | -1 |
| G: -5312.08863 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.81740 HOMO: -6.34570 LUMO: 1.80684 factor:1 | 1 (-0.36308) | -1 | -1 |
| G: -5312.08863 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.81618 HOMO: -6.78380 LUMO: 1.95922 factor:1 | 1 (-0.36186) | -1 | -1 |
| G: -5312.08863 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.95885 HOMO: -6.93618 LUMO: 1.76058 factor:1 | 1 (-0.50453) | -1 | -1 |
| G: -5312.08863 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.83052 HOMO: -6.93346 LUMO: 1.79595 factor:1 | 1 (-0.37620) | -1 | -1 |
| G: -5312.08863 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.01050 HOMO: -6.29671 LUMO: 1.75241 factor:1 | 1 (-0.55617) | -1 | -1 |
| G: -5312.08863 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.80295 HOMO: -6.77019 LUMO: 1.74697 factor:1 | 1 (-0.34863) | -1 | -1 |
| G: -5312.08863 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.01471 HOMO: -6.87360 LUMO: 1.91024 factor:1 | 1 (-0.56039) | -1 | -1 |
| G: -5312.08863 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.19855 HOMO: -6.32665 LUMO: 1.87759 factor:1 | 1 (-0.74423) | -1 | -1 |
| G: -5312.08863 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.72736 HOMO: -6.99877 LUMO: 1.99187 factor:1 | 1 (-0.27304) | -1 | -1 |
| G: -5312.08863 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.88973 HOMO: -6.72665 LUMO: 2.12521 factor:1 | 1 (-0.43541) | -1 | -1 |
| G: -5312.08863 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.88704 HOMO: -6.67767 LUMO: 2.43814 factor:1 | 1 (-0.43272) | -1 | -1 |
| G: -5312.08863 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.73245 HOMO: -6.99605 LUMO: 1.79051 factor:1 | 1 (-0.27813) | -1 | -1 |
| G: -5312.08863 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.97768 HOMO: -6.25046 LUMO: 1.77146 factor:1 | 1 (-0.52336) | -1 | -1 |
| G: -5312.08863 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.81076 HOMO: -6.30488 LUMO: 1.90480 factor:1 | 1 (-0.35644) | -1 | -1 |
| G: -5312.08863 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.05297 HOMO: -6.38379 LUMO: 1.68438 factor:1 | 1 (-0.59865) | -1 | -1 |
| G: -5312.08863 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.90119 HOMO: -6.78924 LUMO: 2.01364 factor:1 | 1 (-0.44687) | -1 | -1 |
| G: -5312.08863 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.74421 HOMO: -6.15249 LUMO: 1.98643 factor:1 | 1 (-0.28988) | -1 | -1 |
| G: -5312.08863 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.64317 HOMO: -6.19331 LUMO: 2.14154 factor:1 | 1 (-0.18885) | -1 | -1 |
| G: -5312.08863 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.00709 HOMO: -6.05998 LUMO: 2.12521 factor:1 | 1 (-0.55277) | -1 | -1 |
| G: -5312.08863 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11578.18804 HOMO: -6.67223 LUMO: 1.91840 factor:1 | 1 (-1.73372) | -1 | -1 |
| G: -5312.08863 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11578.94767 HOMO: -6.79196 LUMO: 2.18507 factor:1 | 1 (-2.49335) | -1 | -1 |
| G: -5312.08863 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11578.05460 HOMO: -6.93346 LUMO: 1.78235 factor:1 | 1 (-1.60027) | -1 | -1 |
| G: -5312.08863 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11578.37251 HOMO: -6.16882 LUMO: 1.80956 factor:1 | 1 (-1.91819) | -1 | -1 |
| G: -5312.08863 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11578.11675 HOMO: -6.72665 LUMO: 2.07895 factor:1 | 1 (-1.66243) | -1 | -1 |
| G: -5312.08863 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.80815 HOMO: -6.73210 LUMO: 1.97827 factor:1 | 1 (-0.35383) | -1 | -1 |
| G: -5312.08863 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.66565 HOMO: -6.84638 LUMO: 1.87214 factor:1 | 1 (-0.21132) | -1 | -1 |
| G: -5312.08863 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.82271 HOMO: -6.83006 LUMO: 2.36195 factor:1 | 1 (-0.36839) | -1 | -1 |
| G: -5312.08863 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.76521 HOMO: -6.97700 LUMO: 1.91024 factor:1 | 1 (-0.31089) | -1 | -1 |
| G: -5312.08863 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.98837 HOMO: -6.20420 LUMO: 1.81772 factor:1 | 1 (-0.53405) | -1 | -1 |
| G: -5312.08863 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.71746 HOMO: -7.09129 LUMO: 2.10344 factor:1 | 1 (-0.26313) | 1 | 1 |
| G: -5312.08863 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.72151 HOMO: -6.77564 LUMO: 2.14970 factor:1 | 1 (-0.26719) | -1 | -1 |
| G: -5312.08863 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.47764 HOMO: -6.81645 LUMO: 1.85854 factor:1 | 1 (-0.02332) | -1 | -1 |
| G: -5312.08863 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.97221 HOMO: -6.50896 LUMO: 2.04358 factor:1 | 1 (-0.51789) | -1 | -1 |
| G: -5312.08863 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.79710 HOMO: -6.89264 LUMO: 1.66262 factor:1 | 1 (-1.34277) | -1 | -1 |
| G: -5312.08863 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11578.39194 HOMO: -6.75931 LUMO: 2.23950 factor:1 | 1 (-1.93761) | -1 | -1 |
| G: -5312.08863 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.66313 HOMO: -6.50080 LUMO: 1.67622 factor:1 | 1 (-1.20881) | -1 | -1 |
| G: -5312.08863 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.80635 HOMO: -6.30216 LUMO: 2.24222 factor:1 | 1 (-1.35202) | -1 | -1 |
| G: -5312.08863 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.96902 HOMO: -7.18108 LUMO: 2.10072 factor:1 | 1 (-1.51469) | 1 | 1 |
| G: -5312.08863 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.70898 HOMO: -6.54162 LUMO: 2.35378 factor:1 | 1 (-1.25466) | -1 | -1 |
| G: -5312.08863 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.65320 HOMO: -5.98650 LUMO: 1.48302 factor:1 | 1 (-1.19888) | -1 | -1 |
| G: -5312.08863 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.97879 HOMO: -7.15115 LUMO: 2.14970 factor:1 | 1 (-1.52446) | 1 | 1 |
| G: -5312.08863 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.60357 HOMO: -6.45454 LUMO: 2.15786 factor:1 | 1 (-1.14925) | -1 | -1 |
| G: -5312.08863 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.78003 HOMO: -7.06952 LUMO: 2.14970 factor:1 | 1 (-1.32571) | 1 | 1 |
| G: -5312.08863 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.99318 HOMO: -6.93618 LUMO: 1.86942 factor:1 | 1 (-1.53886) | -1 | -1 |
| G: -5312.08863 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.89133 HOMO: -6.63141 LUMO: 1.92657 factor:1 | 1 (-1.43701) | -1 | -1 |
| G: -5312.08863 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.64357 HOMO: -6.51441 LUMO: -0.44355 factor:1 | 1 (-1.18925) | -1 | -1 |
| G: -5312.08863 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.71337 HOMO: -6.82734 LUMO: -1.03131 factor:1 | 1 (-1.25904) | -1 | -1 |
| G: -5312.08863 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.56610 HOMO: -6.58788 LUMO: -0.82995 factor:1 | 1 (-1.11178) | -1 | -1 |
| G: -5312.08863 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11578.20581 HOMO: -6.43277 LUMO: -0.40817 factor:1 | 1 (-1.75149) | -1 | -1 |
| G: -5312.08863 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11578.78011 HOMO: -6.78924 LUMO: -0.72110 factor:1 | 1 (-2.32578) | -1 | -1 |
| G: -5312.08863 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11578.16317 HOMO: -7.28177 LUMO: 0.36735 factor:1 | 1 (-1.70885) | -1 | -1 |
| G: -5312.08863 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.93772 HOMO: -6.47903 LUMO: -0.46259 factor:1 | 1 (-1.48340) | -1 | -1 |
| G: -5312.08863 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.96855 HOMO: -6.67495 LUMO: -0.75376 factor:1 | 1 (-1.51423) | -1 | -1 |
| G: -5312.08863 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.74956 HOMO: -6.71033 LUMO: -0.71838 factor:1 | 1 (-1.29523) | -1 | -1 |
| G: -5312.08863 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.61415 HOMO: -6.79740 LUMO: -0.79185 factor:1 | 1 (-1.15983) | -1 | -1 |
| G: -5312.08863 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.65117 HOMO: -6.08719 LUMO: -0.63675 factor:1 | 1 (-0.19685) | -1 | -1 |
| G: -5312.08863 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.87381 HOMO: -6.84094 LUMO: 0.42994 factor:1 | 1 (-0.41949) | -1 | -1 |
| G: -5312.08863 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.86274 HOMO: -6.59604 LUMO: 0.25851 factor:1 | 1 (-0.40842) | -1 | -1 |
| G: -5312.08863 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.77433 HOMO: -6.82462 LUMO: 0.08708 factor:1 | 1 (-0.32001) | -1 | -1 |
| G: -5312.08863 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.75863 HOMO: -6.54706 LUMO: 0.44082 factor:1 | 1 (-0.30430) | -1 | -1 |
| G: -5312.08863 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.69073 HOMO: -6.99333 LUMO: 0.32109 factor:1 | 1 (-0.23641) | -1 | -1 |
| G: -5312.08863 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.88622 HOMO: -6.29944 LUMO: -0.57144 factor:1 | 1 (-0.43190) | -1 | -1 |
| G: -5312.08863 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.68766 HOMO: -6.57699 LUMO: -0.46531 factor:1 | 1 (-0.23334) | -1 | -1 |
| G: -5312.08863 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.96815 HOMO: -6.24773 LUMO: -0.53879 factor:1 | 1 (-0.51383) | -1 | -1 |
| G: -5312.08863 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.72434 HOMO: -6.96067 LUMO: -0.67212 factor:1 | 1 (-0.27002) | -1 | -1 |
| G: -5312.08863 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.81936 HOMO: -7.24095 LUMO: -0.09252 factor:1 | 1 (-0.36504) | -1 | -1 |
| G: -5312.08863 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.56866 HOMO: -6.33481 LUMO: -0.46531 factor:1 | 1 (-0.11434) | -1 | -1 |
| G: -5312.08863 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.96481 HOMO: -6.43549 LUMO: -0.33198 factor:1 | 1 (-0.51049) | -1 | -1 |
| G: -5312.08863 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.69520 HOMO: -6.53073 LUMO: 0.44899 factor:1 | 1 (-0.24088) | -1 | -1 |
| G: -5312.08863 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.60766 HOMO: -6.69128 LUMO: 0.47620 factor:1 | 1 (-0.15334) | -1 | -1 |
| G: -5312.08863 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.55049 HOMO: -6.65318 LUMO: 0.52246 factor:1 | 1 (-0.09617) | -1 | -1 |
| G: -5312.08863 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.70728 HOMO: -6.71305 LUMO: 0.41089 factor:1 | 1 (-0.25296) | -1 | -1 |
| G: -5312.08863 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.79612 HOMO: -6.70216 LUMO: 0.19864 factor:1 | 1 (-0.34180) | -1 | -1 |
| G: -5312.08863 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11578.01846 HOMO: -6.41100 LUMO: 0.34558 factor:1 | 1 (-1.56414) | -1 | -1 |
| G: -5312.08863 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11579.11029 HOMO: -7.01237 LUMO: 0.02993 factor:1 | 1 (-2.65597) | -1 | -1 |
| G: -5312.08863 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11578.18981 HOMO: -6.85999 LUMO: 0.18776 factor:1 | 1 (-1.73549) | -1 | -1 |
| G: -5312.08863 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.64992 HOMO: -6.62869 LUMO: 0.48708 factor:1 | 1 (-0.19560) | -1 | -1 |
| G: -5312.08863 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.78140 HOMO: -6.43821 LUMO: -0.45715 factor:1 | 1 (-0.32708) | -1 | -1 |
| G: -5312.08863 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.79923 HOMO: -6.43277 LUMO: -0.72110 factor:1 | 1 (-0.34490) | -1 | -1 |
| G: -5312.08863 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.64826 HOMO: -7.10761 LUMO: 0.43266 factor:1 | 1 (-0.19394) | -1 | -1 |
| G: -5312.08863 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.81841 HOMO: -6.57699 LUMO: -0.61498 factor:1 | 1 (-0.36409) | -1 | -1 |
| G: -5312.08863 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11578.35662 HOMO: -6.82189 LUMO: -0.75648 factor:1 | 1 (-1.90229) | -1 | -1 |
| G: -5312.08863 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.73696 HOMO: -6.55794 LUMO: -0.67212 factor:1 | 1 (-1.28264) | -1 | -1 |
| G: -5312.08863 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.65111 HOMO: -6.69128 LUMO: 1.88575 factor:1 | 1 (-1.19678) | -1 | -1 |
| G: -5312.08863 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.76719 HOMO: -6.65591 LUMO: 1.70888 factor:1 | 1 (-1.31287) | -1 | -1 |
| G: -5312.08863 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.73451 HOMO: -6.58788 LUMO: 1.68438 factor:1 | 1 (-1.28019) | -1 | -1 |
| G: -5312.08863 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.85348 HOMO: -6.46270 LUMO: 1.72520 factor:1 | 1 (-1.39916) | -1 | -1 |
| G: -5312.08863 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11578.54348 HOMO: -6.57427 LUMO: 1.73881 factor:1 | 1 (-2.08915) | -1 | -1 |
| G: -5312.08863 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.61078 HOMO: -6.45182 LUMO: 1.75241 factor:1 | 1 (-1.15646) | -1 | -1 |
| G: -5312.08863 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.94834 HOMO: -6.51441 LUMO: 1.78779 factor:1 | 1 (-0.49402) | -1 | -1 |
| G: -5312.08863 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.11657 HOMO: -6.67495 LUMO: 2.11705 factor:1 | 1 (-0.66224) | -1 | -1 |
| G: -5312.08863 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.05782 HOMO: -6.22597 LUMO: 1.96466 factor:1 | 1 (-0.60349) | -1 | -1 |
| G: -5312.08863 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.05474 HOMO: -6.68040 LUMO: 2.30753 factor:1 | 1 (-0.60042) | -1 | -1 |
| G: -5312.08863 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.01033 HOMO: -6.65046 LUMO: 2.18235 factor:1 | 1 (-0.55601) | -1 | -1 |
| G: -5312.08863 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.11205 HOMO: -6.38651 LUMO: 1.76874 factor:1 | 1 (-0.65773) | -1 | -1 |
| G: -5312.08863 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.89569 HOMO: -6.41644 LUMO: 2.09256 factor:1 | 1 (-0.44137) | -1 | -1 |
| G: -5312.08863 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.76061 HOMO: -6.14977 LUMO: 2.28031 factor:1 | 1 (-0.30629) | -1 | -1 |
| G: -5312.08863 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.28996 HOMO: -6.70489 LUMO: 2.43814 factor:1 | 1 (-0.83563) | -1 | -1 |
| G: -5312.08863 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.12642 HOMO: -6.78924 LUMO: 2.27215 factor:1 | 1 (-0.67209) | -1 | -1 |
| G: -5312.08863 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.16683 HOMO: -6.86271 LUMO: 2.31025 factor:1 | 1 (-0.71250) | -1 | -1 |
| G: -5312.08863 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.12282 HOMO: -6.51168 LUMO: 2.04630 factor:1 | 1 (-0.66850) | -1 | -1 |
| G: -5312.08863 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.26968 HOMO: -6.72665 LUMO: 2.13337 factor:1 | 1 (-0.81536) | -1 | -1 |
| G: -5312.08863 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.27975 HOMO: -6.45998 LUMO: 2.16058 factor:1 | 1 (-0.82543) | -1 | -1 |
| G: -5312.08863 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.99694 HOMO: -6.83822 LUMO: 2.20684 factor:1 | 1 (-0.54262) | -1 | -1 |
| G: -5312.08863 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.02563 HOMO: -6.68856 LUMO: 2.19324 factor:1 | 1 (-0.57130) | -1 | -1 |
| G: -5312.08863 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.49426 HOMO: -6.71577 LUMO: 2.16058 factor:1 | 1 (-1.03994) | -1 | -1 |
| G: -5312.08863 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.27080 HOMO: -6.82462 LUMO: 1.90208 factor:1 | 1 (-0.81648) | -1 | -1 |
| G: -5312.08863 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.21970 HOMO: -6.61509 LUMO: 2.23950 factor:1 | 1 (-0.76537) | -1 | -1 |
| G: -5312.08863 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.41154 HOMO: -6.73754 LUMO: 1.84221 factor:1 | 1 (-0.95721) | -1 | -1 |
| G: -5312.08863 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.12786 HOMO: -6.56611 LUMO: 1.94561 factor:1 | 1 (-0.67354) | -1 | -1 |
| G: -5312.08863 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.03646 HOMO: -6.67767 LUMO: 1.51840 factor:1 | 1 (-0.58213) | -1 | -1 |
| G: -5312.08863 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.04252 HOMO: -6.35658 LUMO: 2.16603 factor:1 | 1 (-0.58820) | -1 | -1 |
| G: -5312.08863 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.17208 HOMO: -6.35114 LUMO: 2.08983 factor:1 | 1 (-0.71775) | -1 | -1 |
| G: -5312.08863 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.27534 HOMO: -6.35114 LUMO: 2.10616 factor:1 | 1 (-0.82102) | -1 | -1 |
| G: -5312.08863 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.19602 HOMO: -6.71305 LUMO: 2.01636 factor:1 | 1 (-0.74170) | -1 | -1 |
| G: -5312.08863 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.34925 HOMO: -6.24773 LUMO: 1.98915 factor:1 | 1 (-0.89493) | -1 | -1 |
| G: -5312.08863 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.23695 HOMO: -6.53617 LUMO: 2.42726 factor:1 | 1 (-0.78263) | -1 | -1 |
| G: -5312.08863 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.24002 HOMO: -6.59332 LUMO: 1.82316 factor:1 | 1 (-0.78570) | -1 | -1 |
| G: -5312.08863 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.05303 HOMO: -6.41372 LUMO: 1.77418 factor:1 | 1 (-0.59870) | -1 | -1 |
| G: -5312.08863 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.00054 HOMO: -6.40284 LUMO: 1.88575 factor:1 | 1 (-0.54621) | -1 | -1 |
| G: -5312.08863 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.78951 HOMO: -6.11168 LUMO: 1.70888 factor:1 | 1 (-0.33519) | -1 | -1 |
| G: -5312.08863 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.03101 HOMO: -6.44910 LUMO: 2.23405 factor:1 | 1 (-0.57669) | -1 | -1 |
| G: -5312.08863 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.20609 HOMO: -6.24773 LUMO: 2.12793 factor:1 | 1 (-0.75177) | -1 | -1 |
| G: -5312.08863 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.03836 HOMO: -6.07358 LUMO: 1.89663 factor:1 | 1 (-0.58404) | -1 | -1 |
| G: -5312.08863 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.91520 HOMO: -6.66679 LUMO: 1.96738 factor:1 | 1 (-0.46088) | -1 | -1 |
| G: -5312.08863 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.18606 HOMO: -6.68312 LUMO: 1.78235 factor:1 | 1 (-0.73174) | -1 | -1 |
| G: -5312.08863 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.73112 HOMO: -6.70761 LUMO: 1.97555 factor:1 | 1 (-0.27679) | -1 | -1 |
| G: -5312.08863 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.61925 HOMO: -6.15794 LUMO: 2.00548 factor:1 | 1 (-0.16493) | -1 | -1 |
| G: -5312.08863 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: 1.96738 factor:1 | 1 (-0.63332) | -1 | -1 |
| G: -5312.08863 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.22753 HOMO: -6.25590 LUMO: 1.86670 factor:1 | 1 (-0.77321) | -1 | -1 |
| G: -5312.08863 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.01792 HOMO: -6.30216 LUMO: 1.84765 factor:1 | 1 (-0.56360) | -1 | -1 |
| G: -5312.08863 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.30457 HOMO: -6.76747 LUMO: 2.20956 factor:1 | 1 (-0.85025) | -1 | -1 |
| G: -5312.08863 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.11387 HOMO: -6.14161 LUMO: 1.80684 factor:1 | 1 (-0.65955) | -1 | -1 |
| G: -5312.08863 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.87577 HOMO: -6.81373 LUMO: 1.91024 factor:1 | 1 (-0.42145) | -1 | -1 |
| G: -5312.08863 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.67611 HOMO: -6.81917 LUMO: 2.34834 factor:1 | 1 (-1.22179) | -1 | -1 |
| G: -5312.08863 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.67802 HOMO: -6.72121 LUMO: 1.90208 factor:1 | 1 (-1.22370) | -1 | -1 |
| G: -5312.08863 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.99155 HOMO: -7.51851 LUMO: 0.26939 factor:1 | 1 (-1.53723) | -1 | -1 |
| G: -5312.08863 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.90575 HOMO: -6.65318 LUMO: -0.57144 factor:1 | 1 (-1.45143) | -1 | -1 |
| G: -5312.08863 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.85865 HOMO: -6.77564 LUMO: -0.72654 factor:1 | 1 (-1.40433) | -1 | -1 |
| G: -5312.08863 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.81416 HOMO: -6.80557 LUMO: -0.60954 factor:1 | 1 (-1.35983) | -1 | -1 |
| G: -5312.08863 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11578.01541 HOMO: -7.35524 LUMO: 0.27483 factor:1 | 1 (-1.56109) | -1 | -1 |
| G: -5312.08863 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11578.09452 HOMO: -6.94979 LUMO: -0.83811 factor:1 | 1 (-1.64019) | -1 | -1 |
| G: -5312.08863 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.90474 HOMO: -6.13345 LUMO: -0.67212 factor:1 | 1 (-1.45042) | -1 | -1 |
| G: -5312.08863 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.85944 HOMO: -6.47359 LUMO: -0.59321 factor:1 | 1 (-1.40511) | -1 | -1 |
| G: -5312.08863 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.87750 HOMO: -6.52257 LUMO: -0.54695 factor:1 | 1 (-1.42318) | -1 | -1 |
| G: -5312.08863 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.94532 HOMO: -6.61781 LUMO: -0.69661 factor:1 | 1 (-1.49099) | -1 | -1 |
| G: -5312.08863 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.53225 HOMO: -6.77564 LUMO: -0.80001 factor:1 | 1 (-1.07792) | -1 | -1 |
| G: -5312.08863 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.52909 HOMO: -7.35252 LUMO: -1.00410 factor:1 | 1 (-1.07477) | -1 | -1 |
| G: -5312.08863 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.18925 HOMO: -6.35386 LUMO: -0.38912 factor:1 | 1 (-0.73493) | -1 | -1 |
| G: -5312.08863 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.09014 HOMO: -6.80285 LUMO: -0.52246 factor:1 | 1 (-0.63582) | -1 | -1 |
| G: -5312.08863 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.02601 HOMO: -7.23279 LUMO: 0.30477 factor:1 | 1 (-0.57168) | -1 | -1 |
| G: -5312.08863 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.12761 HOMO: -7.13483 LUMO: -0.76192 factor:1 | 1 (-0.67329) | -1 | -1 |
| G: -5312.08863 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.23515 HOMO: -6.71849 LUMO: -0.48164 factor:1 | 1 (-0.78083) | -1 | -1 |
| G: -5312.08863 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.42912 HOMO: -6.85455 LUMO: -0.69389 factor:1 | 1 (-0.97479) | -1 | -1 |
| G: -5312.08863 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.25564 HOMO: -6.96339 LUMO: -0.73743 factor:1 | 1 (-0.80132) | -1 | -1 |
| G: -5312.08863 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.07262 HOMO: -7.50490 LUMO: 0.28844 factor:1 | 1 (-0.61830) | -1 | -1 |
| G: -5312.08863 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.96851 HOMO: -6.63958 LUMO: -0.50069 factor:1 | 1 (-0.51419) | -1 | -1 |
| G: -5312.08863 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.64830 HOMO: -6.78924 LUMO: -0.69661 factor:1 | 1 (-1.19398) | -1 | -1 |
| G: -5312.08863 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.78792 HOMO: -7.44776 LUMO: 0.33742 factor:1 | 1 (-1.33360) | -1 | -1 |
| G: -5312.08863 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.77935 HOMO: -6.15249 LUMO: 0.66396 factor:1 | 1 (-1.32503) | -1 | -1 |
| G: -5312.08863 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.48000 HOMO: -6.17426 LUMO: 0.55511 factor:1 | 1 (-1.02568) | -1 | -1 |
| G: -5312.08863 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.60520 HOMO: -6.83550 LUMO: 0.28844 factor:1 | 1 (-1.15088) | -1 | -1 |
| G: -5312.08863 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.52966 HOMO: -6.32393 LUMO: 0.47620 factor:1 | 1 (-1.07534) | -1 | -1 |
| G: -5312.08863 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.73465 HOMO: -6.32937 LUMO: 0.45987 factor:1 | 1 (-1.28032) | -1 | -1 |
| G: -5312.08863 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.79674 HOMO: -7.37429 LUMO: 0.09252 factor:1 | 1 (-1.34242) | -1 | -1 |
| G: -5312.08863 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.89661 HOMO: -6.54434 LUMO: -0.39729 factor:1 | 1 (-1.44229) | -1 | -1 |
| G: -5312.08863 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.76188 HOMO: -7.35524 LUMO: 0.28028 factor:1 | 1 (-1.30756) | -1 | -1 |
| G: -5312.08863 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.63121 HOMO: -6.95523 LUMO: -0.86804 factor:1 | 1 (-1.17689) | -1 | -1 |
| G: -5312.08863 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.66942 HOMO: -6.63958 LUMO: -0.65307 factor:1 | 1 (-1.21510) | -1 | -1 |
| G: -5312.08863 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.44680 HOMO: -6.73482 LUMO: -0.67212 factor:1 | 1 (-0.99248) | -1 | -1 |
| G: -5312.08863 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.38041 HOMO: -6.37835 LUMO: -0.53606 factor:1 | 1 (-0.92609) | -1 | -1 |
| G: -5312.08863 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.87582 HOMO: -6.71849 LUMO: -0.61226 factor:1 | 1 (-1.42150) | -1 | -1 |
| G: -5312.08863 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.78741 HOMO: -6.68584 LUMO: -1.11022 factor:1 | 1 (-1.33309) | -1 | -1 |
| G: -5312.08863 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.57883 HOMO: -6.80285 LUMO: -0.79185 factor:1 | 1 (-1.12451) | -1 | -1 |
| G: -5312.08863 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.53548 HOMO: -7.14571 LUMO: -0.94696 factor:1 | 1 (-1.08116) | -1 | -1 |
| G: -5312.08863 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.71884 HOMO: -7.16204 LUMO: -0.66124 factor:1 | 1 (-1.26451) | -1 | -1 |
| G: -5312.08863 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.56027 HOMO: -6.54978 LUMO: -0.54967 factor:1 | 1 (-1.10595) | -1 | -1 |
| G: -5312.08863 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.60539 HOMO: -6.75114 LUMO: -0.70750 factor:1 | 1 (-1.15107) | -1 | -1 |
| G: -5312.08863 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.86542 HOMO: -7.22190 LUMO: 0.39184 factor:1 | 1 (-1.41110) | -1 | -1 |
| G: -5312.08863 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.84153 HOMO: -7.43959 LUMO: 0.30477 factor:1 | 1 (-1.38721) | -1 | -1 |
| G: -5312.08863 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.79122 HOMO: -6.87360 LUMO: -0.77552 factor:1 | 1 (-1.33690) | -1 | -1 |
| G: -5312.08863 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.86757 HOMO: -6.82734 LUMO: -0.59593 factor:1 | 1 (-1.41325) | -1 | -1 |
| G: -5312.08863 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.44610 HOMO: -6.65318 LUMO: -0.46259 factor:1 | 1 (-0.99177) | -1 | -1 |
| G: -5312.08863 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.48253 HOMO: -7.05863 LUMO: -1.17009 factor:1 | 1 (-1.02821) | -1 | -1 |
| G: -5312.08863 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11578.00534 HOMO: -6.57427 LUMO: -0.48708 factor:1 | 1 (-1.55102) | -1 | -1 |
| G: -5312.08863 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.02437 HOMO: -6.60420 LUMO: -0.38096 factor:1 | 1 (-0.57005) | -1 | -1 |
| G: -5312.08863 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.83112 HOMO: -6.72121 LUMO: -0.66668 factor:1 | 1 (-0.37680) | -1 | -1 |
| G: -5312.08863 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.03741 HOMO: -6.52257 LUMO: -0.19320 factor:1 | 1 (-0.58309) | -1 | -1 |
| G: -5312.08863 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.16111 HOMO: -6.28039 LUMO: -0.27211 factor:1 | 1 (-0.70679) | -1 | -1 |
| G: -5312.08863 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.77963 HOMO: -6.71849 LUMO: -0.42722 factor:1 | 1 (-0.32531) | -1 | -1 |
| G: -5312.08863 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.97368 HOMO: -6.27495 LUMO: 0.27756 factor:1 | 1 (-0.51936) | -1 | -1 |
| G: -5312.08863 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.91398 HOMO: -6.21780 LUMO: 0.46531 factor:1 | 1 (-0.45965) | -1 | -1 |
| G: -5312.08863 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.86132 HOMO: -6.52257 LUMO: -0.64491 factor:1 | 1 (-0.40700) | -1 | -1 |
| G: -5312.08863 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.74589 HOMO: -6.73754 LUMO: 1.83133 factor:1 | 1 (-0.29157) | -1 | -1 |
| G: -5312.08863 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.68246 HOMO: -6.67223 LUMO: 1.88847 factor:1 | 1 (-0.22814) | -1 | -1 |
| G: -5312.08863 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.05036 HOMO: -6.82189 LUMO: 1.59187 factor:1 | 1 (-0.59604) | -1 | -1 |
| G: -5312.08863 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.90026 HOMO: -6.43277 LUMO: 1.76330 factor:1 | 1 (-0.44594) | -1 | -1 |
| G: -5312.08863 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.29856 HOMO: -6.48175 LUMO: 1.77962 factor:1 | 1 (-0.84423) | -1 | -1 |
| G: -5312.08863 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.01833 HOMO: -6.50352 LUMO: 1.68438 factor:1 | 1 (-0.56401) | -1 | -1 |
| G: -5312.08863 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.92728 HOMO: -6.31576 LUMO: 2.03813 factor:1 | 1 (-0.47296) | -1 | -1 |
| G: -5312.08863 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.89828 HOMO: -6.27495 LUMO: 1.99459 factor:1 | 1 (-0.44395) | -1 | -1 |
| G: -5312.08863 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.85180 HOMO: -6.23957 LUMO: 2.17147 factor:1 | 1 (-0.39748) | -1 | -1 |
| G: -5312.08863 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.98070 HOMO: -6.78108 LUMO: 2.16875 factor:1 | 1 (-0.52638) | -1 | -1 |
| G: -5312.08863 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.20810 HOMO: -6.34297 LUMO: 2.10344 factor:1 | 1 (-0.75378) | -1 | -1 |
| G: -5312.08863 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.69237 HOMO: -6.30216 LUMO: 2.00004 factor:1 | 1 (-0.23805) | -1 | -1 |
| G: -5312.08863 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.96824 HOMO: -6.72665 LUMO: 2.09528 factor:1 | 1 (-0.51391) | -1 | -1 |
| G: -5312.08863 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.09997 HOMO: -6.86543 LUMO: 1.91568 factor:1 | 1 (-0.64564) | -1 | -1 |
| G: -5312.08863 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.91844 HOMO: -5.83956 LUMO: 1.89391 factor:1 | 1 (-0.46412) | -1 | -1 |
| G: -5312.08863 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.90443 HOMO: -6.42189 LUMO: 2.03269 factor:1 | 1 (-0.45010) | -1 | -1 |
| G: -5312.08863 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.82214 HOMO: -6.07630 LUMO: 1.80956 factor:1 | 1 (-0.36782) | -1 | -1 |
| G: -5312.08863 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.06573 HOMO: -6.43277 LUMO: 1.81772 factor:1 | 1 (-0.61141) | -1 | -1 |
| G: -5312.08863 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.81558 HOMO: -7.03959 LUMO: 1.78779 factor:1 | 1 (-0.36126) | -1 | -1 |
| G: -5312.08863 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.76570 HOMO: -6.72121 LUMO: 2.29664 factor:1 | 1 (-0.31138) | -1 | -1 |
| G: -5312.08863 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.68400 HOMO: -6.62869 LUMO: 2.04630 factor:1 | 1 (-1.22968) | -1 | -1 |
| G: -5312.08863 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.88300 HOMO: -6.63958 LUMO: 1.84221 factor:1 | 1 (-1.42868) | -1 | -1 |
| G: -5312.08863 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.80422 HOMO: -6.70761 LUMO: 1.67350 factor:1 | 1 (-1.34990) | -1 | -1 |
| G: -5312.08863 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.33064 HOMO: -6.00283 LUMO: 1.64357 factor:1 | 1 (-0.87632) | -1 | -1 |
| G: -5312.08863 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.75894 HOMO: -6.48719 LUMO: 1.70343 factor:1 | 1 (-1.30462) | -1 | -1 |
| G: -5312.08863 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.47532 HOMO: -6.13345 LUMO: 1.44492 factor:1 | 1 (-1.02100) | -1 | -1 |
| G: -5312.08863 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.45513 HOMO: -6.11168 LUMO: 1.70071 factor:1 | 1 (-1.00081) | -1 | -1 |
| G: -5312.08863 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.65290 HOMO: -6.09535 LUMO: 1.82316 factor:1 | 1 (-1.19858) | -1 | -1 |
| G: -5312.08863 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.93150 HOMO: -6.81101 LUMO: 1.63540 factor:1 | 1 (-0.47718) | -1 | -1 |
| G: -5312.08863 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.92059 HOMO: -6.80013 LUMO: 2.12249 factor:1 | 1 (-0.46627) | -1 | -1 |
| G: -5312.08863 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.20541 HOMO: -6.48447 LUMO: 1.94561 factor:1 | 1 (-0.75109) | -1 | -1 |
| G: -5312.08863 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.73593 HOMO: -6.72393 LUMO: 2.06534 factor:1 | 1 (-0.28161) | -1 | -1 |
| G: -5312.08863 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.74094 HOMO: -6.34570 LUMO: 1.98915 factor:1 | 1 (-0.28662) | -1 | -1 |
| G: -5312.08863 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.04489 HOMO: -6.31304 LUMO: 1.87759 factor:1 | 1 (-0.59057) | -1 | -1 |
| G: -5312.08863 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.92568 HOMO: -6.77564 LUMO: 1.81228 factor:1 | 1 (-0.47136) | -1 | -1 |
| G: -5312.08863 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.98187 HOMO: -6.58516 LUMO: 2.34834 factor:1 | 1 (-0.52755) | -1 | -1 |
| G: -5312.08863 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.27722 HOMO: -6.68040 LUMO: 2.20412 factor:1 | 1 (-0.82290) | -1 | -1 |
| G: -5312.08863 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.82358 HOMO: -6.20964 LUMO: 2.17147 factor:1 | 1 (-0.36926) | -1 | -1 |
| G: -5312.08863 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.57054 HOMO: -6.54706 LUMO: 2.03813 factor:1 | 1 (-0.11622) | -1 | -1 |
| G: -5312.08863 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.08184 HOMO: -6.54162 LUMO: 2.17419 factor:1 | 1 (-0.62752) | -1 | -1 |
| G: -5312.08863 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.70129 HOMO: -6.75659 LUMO: 2.22589 factor:1 | 1 (-0.24697) | -1 | -1 |
| G: -5312.08863 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.94511 HOMO: -6.59604 LUMO: 2.59325 factor:1 | 1 (-0.49078) | -1 | -1 |
| G: -5312.08863 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.06628 HOMO: -6.11712 LUMO: 2.02181 factor:1 | 1 (-0.61196) | -1 | -1 |
| G: -5312.08863 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.78309 HOMO: -6.63141 LUMO: 2.09256 factor:1 | 1 (-0.32877) | -1 | -1 |
| G: -5312.08863 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.83762 HOMO: -6.61781 LUMO: 1.86126 factor:1 | 1 (-0.38330) | -1 | -1 |
| G: -5312.08863 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.66676 HOMO: -6.63958 LUMO: 1.77146 factor:1 | 1 (-0.21244) | -1 | -1 |
| G: -5312.08863 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.03112 HOMO: -6.60420 LUMO: 1.54561 factor:1 | 1 (-0.57680) | -1 | -1 |
| G: -5312.08863 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.22819 HOMO: -6.52529 LUMO: 2.05174 factor:1 | 1 (-0.77386) | -1 | -1 |
| G: -5312.08863 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.85466 HOMO: -6.80285 LUMO: 2.13609 factor:1 | 1 (-0.40033) | -1 | -1 |
| G: -5312.08863 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.01031 HOMO: -6.51168 LUMO: 2.25855 factor:1 | 1 (-0.55598) | -1 | -1 |
| G: -5312.08863 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.97088 HOMO: -6.64774 LUMO: 2.46263 factor:1 | 1 (-0.51655) | -1 | -1 |
| G: -5312.08863 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.19308 HOMO: -6.40828 LUMO: 1.99732 factor:1 | 1 (-0.73876) | -1 | -1 |
| G: -5312.08863 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.08269 HOMO: -5.97562 LUMO: 1.56465 factor:1 | 1 (-0.62837) | -1 | -1 |
| G: -5312.08863 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.92135 HOMO: -6.75659 LUMO: 2.23405 factor:1 | 1 (-0.46703) | -1 | -1 |
| G: -5312.08863 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.92456 HOMO: -6.68584 LUMO: 2.09528 factor:1 | 1 (-0.47024) | -1 | -1 |
| G: -5312.08863 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.84701 HOMO: -6.86543 LUMO: 1.95106 factor:1 | 1 (-0.39269) | -1 | -1 |
| G: -5312.08863 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.89330 HOMO: -6.47359 LUMO: 1.82316 factor:1 | 1 (-0.43897) | -1 | -1 |
| G: -5312.08863 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.72197 HOMO: -6.87632 LUMO: 2.08439 factor:1 | 1 (-0.26765) | -1 | -1 |
| G: -5312.08863 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.94451 HOMO: -6.33753 LUMO: 2.16603 factor:1 | 1 (-0.49019) | -1 | -1 |
| G: -5312.08863 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.79626 HOMO: -6.92258 LUMO: 1.72248 factor:1 | 1 (-0.34194) | -1 | -1 |
| G: -5312.08863 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.07939 HOMO: -6.62597 LUMO: 2.10344 factor:1 | 1 (-0.62507) | -1 | -1 |
| G: -5312.08863 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.96478 HOMO: -6.63141 LUMO: 1.94017 factor:1 | 1 (-0.51046) | -1 | -1 |
| G: -5312.08863 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.76636 HOMO: -6.48447 LUMO: 1.91840 factor:1 | 1 (-0.31203) | -1 | -1 |
| G: -5312.08863 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.13714 HOMO: -6.41372 LUMO: 1.61364 factor:1 | 1 (-0.68282) | -1 | -1 |
| G: -5312.08863 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.75381 HOMO: -6.37291 LUMO: 1.79051 factor:1 | 1 (-0.29949) | -1 | -1 |
| G: -5312.08863 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.68619 HOMO: -6.13073 LUMO: 1.77962 factor:1 | 1 (-0.23187) | -1 | -1 |
| G: -5312.08863 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.49944 HOMO: -6.13073 LUMO: 1.98915 factor:1 | 1 (-0.04512) | -1 | -1 |
| G: -5312.08863 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.92116 HOMO: -6.44094 LUMO: 1.58370 factor:1 | 1 (-0.46684) | -1 | -1 |
| G: -5312.08863 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.03504 HOMO: -6.87087 LUMO: -0.82995 factor:1 | 1 (-0.58072) | -1 | -1 |
| G: -5312.08863 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.07667 HOMO: -6.67223 LUMO: 1.08029 factor:1 | 1 (-0.62235) | -1 | -1 |
| G: -5312.08863 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.74293 HOMO: -6.82462 LUMO: 0.91702 factor:1 | 1 (-0.28860) | -1 | -1 |
| G: -5312.08863 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.64899 HOMO: -6.65863 LUMO: 1.52656 factor:1 | 1 (-0.19467) | -1 | -1 |
| G: -5312.08863 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.11213 HOMO: -6.78924 LUMO: 0.86260 factor:1 | 1 (-0.65781) | -1 | -1 |
| G: -5312.08863 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.13232 HOMO: -6.68584 LUMO: 0.94424 factor:1 | 1 (-0.67800) | -1 | -1 |
| G: -5312.08863 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.21714 HOMO: -6.58788 LUMO: 1.00138 factor:1 | 1 (-0.76282) | -1 | -1 |
| G: -5312.08863 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.27488 HOMO: -6.79740 LUMO: 0.91430 factor:1 | 1 (-0.82056) | -1 | -1 |
| G: -5312.08863 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.01229 HOMO: -6.67223 LUMO: 0.80274 factor:1 | 1 (-0.55797) | -1 | -1 |
| G: -5312.08863 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.12990 HOMO: -6.95251 LUMO: 0.90614 factor:1 | 1 (-0.67558) | -1 | -1 |
| G: -5312.08863 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.98062 HOMO: -7.19469 LUMO: 1.34152 factor:1 | 1 (-0.52630) | -1 | -1 |
| G: -5312.08863 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.63745 HOMO: -6.59332 LUMO: -0.76464 factor:1 | 1 (-1.18312) | -1 | -1 |
| G: -5312.08863 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.52874 HOMO: -6.77564 LUMO: -0.90886 factor:1 | 1 (-1.07441) | -1 | -1 |
| G: -5312.08863 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.70515 HOMO: -6.57971 LUMO: -0.41633 factor:1 | 1 (-1.25083) | -1 | -1 |
| G: -5312.08863 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.89748 HOMO: -6.68856 LUMO: -0.58232 factor:1 | 1 (-1.44316) | -1 | -1 |
| G: -5312.08863 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.57842 HOMO: -6.87087 LUMO: -0.71022 factor:1 | 1 (-1.12410) | -1 | -1 |
| G: -5312.08863 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.45472 HOMO: -6.67767 LUMO: -0.74559 factor:1 | 1 (-1.00040) | -1 | -1 |
| G: -5312.08863 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.96644 HOMO: -6.68040 LUMO: -0.65307 factor:1 | 1 (-0.51212) | -1 | -1 |
| G: -5312.08863 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.98712 HOMO: -6.32937 LUMO: 0.80274 factor:1 | 1 (-0.53280) | -1 | -1 |
| G: -5312.08863 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.79120 HOMO: -6.29671 LUMO: 0.82723 factor:1 | 1 (-0.33688) | -1 | -1 |
| G: -5312.08863 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.68412 HOMO: -6.67767 LUMO: 0.59321 factor:1 | 1 (-0.22980) | -1 | -1 |
| G: -5312.08863 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.41359 HOMO: -6.77836 LUMO: 0.50341 factor:1 | -1 (0.04074) | -1 | -1 |
| G: -5312.08863 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.86970 HOMO: -6.61781 LUMO: 0.42450 factor:1 | 1 (-0.41538) | -1 | -1 |
| G: -5312.08863 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.60431 HOMO: -6.83278 LUMO: 0.39457 factor:1 | 1 (-0.14999) | -1 | -1 |
| G: -5312.08863 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.29957 HOMO: -6.56883 LUMO: 0.64219 factor:1 | -1 (0.15475) | -1 | -1 |
| G: -5312.08863 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.16326 HOMO: -6.71577 LUMO: 0.40001 factor:1 | 1 (-0.70894) | -1 | -1 |
| G: -5312.08863 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.08745 HOMO: -6.86543 LUMO: -0.74287 factor:1 | 1 (-0.63313) | -1 | -1 |
| G: -5312.08863 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.26451 HOMO: -6.68584 LUMO: -0.69389 factor:1 | 1 (-0.81019) | -1 | -1 |
| G: -5312.08863 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.38332 HOMO: -6.61237 LUMO: -0.48980 factor:1 | 1 (-0.92900) | -1 | -1 |
| G: -5312.08863 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.39948 HOMO: -6.80285 LUMO: -0.58232 factor:1 | 1 (-0.94516) | -1 | -1 |
| G: -5312.08863 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.03632 HOMO: -6.88992 LUMO: -0.70205 factor:1 | 1 (-0.58200) | -1 | -1 |
| G: -5312.08863 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.09812 HOMO: -6.95251 LUMO: -0.71838 factor:1 | 1 (-0.64379) | -1 | -1 |
| G: -5312.08863 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.94685 HOMO: -7.52123 LUMO: 0.27211 factor:1 | 1 (-0.49253) | -1 | -1 |
| G: -5312.08863 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.28601 HOMO: -6.76747 LUMO: -0.74015 factor:1 | 1 (-0.83169) | -1 | -1 |
| G: -5312.08863 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.99713 HOMO: -6.55250 LUMO: -0.49797 factor:1 | 1 (-0.54281) | -1 | -1 |
| G: -5312.08863 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.09074 HOMO: -6.50896 LUMO: -0.46804 factor:1 | 1 (-0.63642) | -1 | -1 |
| G: -5312.08863 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.34656 HOMO: -7.45320 LUMO: 0.08436 factor:1 | 1 (-0.89223) | -1 | -1 |
| G: -5312.08863 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.19115 HOMO: -6.82462 LUMO: -0.70477 factor:1 | 1 (-0.73683) | -1 | -1 |
| G: -5312.08863 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.84086 HOMO: -6.57155 LUMO: -0.43538 factor:1 | 1 (-0.38654) | -1 | -1 |
| G: -5312.08863 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.68709 HOMO: -6.72665 LUMO: -0.55239 factor:1 | 1 (-0.23277) | -1 | -1 |
| G: -5312.08863 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.80132 HOMO: -7.05319 LUMO: -1.08573 factor:1 | 1 (-0.34700) | -1 | -1 |
| G: -5312.08863 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.69625 HOMO: -6.56067 LUMO: -0.45715 factor:1 | 1 (-1.24193) | -1 | -1 |
| G: -5312.08863 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.81827 HOMO: -6.76475 LUMO: -0.53879 factor:1 | 1 (-1.36394) | -1 | -1 |
| G: -5312.08863 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.88526 HOMO: -6.67223 LUMO: -0.45987 factor:1 | 1 (-1.43094) | -1 | -1 |
| G: -5312.08863 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.88980 HOMO: -6.44094 LUMO: -0.72110 factor:1 | 1 (-1.43548) | -1 | -1 |
| G: -5312.08863 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11578.06652 HOMO: -6.66951 LUMO: -0.67756 factor:1 | 1 (-1.61219) | -1 | -1 |
| G: -5312.08863 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.83829 HOMO: -6.69400 LUMO: -0.62858 factor:1 | 1 (-1.38397) | -1 | -1 |
| G: -5312.08863 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.65535 HOMO: -6.51985 LUMO: -0.37007 factor:1 | 1 (-1.20103) | -1 | -1 |
| G: -5312.08863 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.04835 HOMO: -5.98378 LUMO: 0.78641 factor:1 | 1 (-0.59402) | -1 | -1 |
| G: -5312.08863 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.15640 HOMO: -6.11440 LUMO: 0.71294 factor:1 | 1 (-0.70208) | -1 | -1 |
| G: -5312.08863 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.17488 HOMO: -6.45182 LUMO: 0.63947 factor:1 | 1 (-0.72056) | -1 | -1 |
| G: -5312.08863 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.31189 HOMO: -6.78924 LUMO: 0.37007 factor:1 | 1 (-0.85757) | -1 | -1 |
| G: -5312.08863 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.35012 HOMO: -6.63686 LUMO: 0.54423 factor:1 | 1 (-0.89580) | -1 | -1 |
| G: -5312.08863 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.09091 HOMO: -6.66679 LUMO: 0.48708 factor:1 | 1 (-0.63658) | -1 | -1 |
| G: -5312.08863 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.99406 HOMO: -6.81917 LUMO: 0.31021 factor:1 | 1 (-0.53974) | -1 | -1 |
| G: -5312.08863 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.75104 HOMO: -6.28583 LUMO: 0.44899 factor:1 | 1 (-0.29671) | -1 | -1 |
| G: -5312.08863 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.06114 HOMO: -6.61237 LUMO: 0.49525 factor:1 | 1 (-0.60681) | -1 | -1 |
| G: -5312.08863 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.94192 HOMO: -7.08857 LUMO: 0.38368 factor:1 | 1 (-0.48760) | -1 | -1 |
| G: -5312.08863 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.88837 HOMO: -6.53890 LUMO: -0.68845 factor:1 | 1 (-0.43405) | -1 | -1 |
| G: -5312.08863 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.07659 HOMO: -6.56611 LUMO: -0.66396 factor:1 | 1 (-0.62227) | -1 | -1 |
| G: -5312.08863 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.91991 HOMO: -6.04909 LUMO: -0.59865 factor:1 | 1 (-0.46559) | -1 | -1 |
| G: -5312.08863 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.06304 HOMO: -6.74842 LUMO: -0.77825 factor:1 | 1 (-0.60872) | -1 | -1 |
| G: -5312.08863 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.96138 HOMO: -6.82462 LUMO: -0.61498 factor:1 | 1 (-0.50706) | -1 | -1 |
| G: -5312.08863 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.70750 HOMO: -7.40694 LUMO: 0.32926 factor:1 | 1 (-0.25317) | -1 | -1 |
| G: -5312.08863 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.84739 HOMO: -6.80557 LUMO: -0.57416 factor:1 | 1 (-0.39307) | -1 | -1 |
| G: -5312.08863 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.58676 HOMO: -6.76747 LUMO: -0.67484 factor:1 | 1 (-0.13244) | -1 | -1 |
| G: -5312.08863 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.81666 HOMO: -7.23279 LUMO: 0.48980 factor:1 | 1 (-1.36234) | -1 | -1 |
| G: -5312.08863 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.73437 HOMO: -6.62869 LUMO: -0.24762 factor:1 | 1 (-1.28005) | -1 | -1 |
| G: -5312.08863 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.79914 HOMO: -6.65863 LUMO: -0.28028 factor:1 | 1 (-1.34481) | -1 | -1 |
| G: -5312.08863 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.63399 HOMO: -6.50352 LUMO: -0.44899 factor:1 | 1 (-1.17967) | -1 | -1 |
| G: -5312.08863 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.89179 HOMO: -6.62053 LUMO: -0.88437 factor:1 | 1 (-1.43747) | -1 | -1 |
| G: -5312.08863 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.87125 HOMO: -6.73754 LUMO: -0.77825 factor:1 | 1 (-1.41692) | -1 | -1 |
| G: -5312.08863 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11578.06064 HOMO: -7.24639 LUMO: 0.35647 factor:1 | 1 (-1.60632) | -1 | -1 |
| G: -5312.08863 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.61208 HOMO: -6.46270 LUMO: -0.48164 factor:1 | 1 (-1.15776) | -1 | -1 |
| G: -5312.08863 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.62373 HOMO: -6.14161 LUMO: -0.66396 factor:1 | 1 (-1.16941) | -1 | -1 |
| G: -5312.08863 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.53227 HOMO: -6.63414 LUMO: 1.51295 factor:1 | 1 (-1.07795) | -1 | -1 |
| G: -5312.08863 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.94232 HOMO: -6.52529 LUMO: 1.65989 factor:1 | 1 (-1.48800) | -1 | -1 |
| G: -5312.08863 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.12125 HOMO: -6.63686 LUMO: 1.64629 factor:1 | 1 (-0.66692) | -1 | -1 |
| G: -5312.08863 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.03354 HOMO: -6.49808 LUMO: 1.60003 factor:1 | 1 (-0.57922) | -1 | -1 |
| G: -5312.08863 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.34838 HOMO: -6.85183 LUMO: 1.96194 factor:1 | 1 (-0.89406) | -1 | -1 |
| G: -5312.08863 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.90081 HOMO: -6.90081 LUMO: 1.82316 factor:1 | 1 (-0.44648) | -1 | -1 |
| G: -5312.08863 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.73860 HOMO: -6.20147 LUMO: 1.95106 factor:1 | 1 (-0.28428) | -1 | -1 |
| G: -5312.08863 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.93972 HOMO: -7.05047 LUMO: 1.94289 factor:1 | 1 (-0.48540) | -1 | -1 |
| G: -5312.08863 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.95477 HOMO: -6.11440 LUMO: 1.83949 factor:1 | 1 (-0.50044) | -1 | -1 |
| G: -5312.08863 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.23238 HOMO: -6.65046 LUMO: 1.59187 factor:1 | 1 (-0.77806) | -1 | -1 |
| G: -5312.08863 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.09940 HOMO: -6.81917 LUMO: 2.41365 factor:1 | 1 (-0.64507) | -1 | -1 |
| G: -5312.08863 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.70935 HOMO: -6.40284 LUMO: 2.48984 factor:1 | 1 (-0.25503) | -1 | -1 |
| G: -5312.08863 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.63765 HOMO: -7.04775 LUMO: 2.31025 factor:1 | 1 (-0.18332) | -1 | -1 |
| G: -5312.08863 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.10530 HOMO: -6.64774 LUMO: 2.20140 factor:1 | 1 (-0.65098) | -1 | -1 |
| G: -5312.08863 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.99441 HOMO: -6.72393 LUMO: 2.28304 factor:1 | 1 (-0.54009) | -1 | -1 |
| G: -5312.08863 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.93267 HOMO: -6.35114 LUMO: 1.84765 factor:1 | 1 (-0.47835) | -1 | -1 |
| G: -5312.08863 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.20152 HOMO: -6.41100 LUMO: 1.74697 factor:1 | 1 (-0.74720) | -1 | -1 |
| G: -5312.08863 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.25621 HOMO: -6.34297 LUMO: 1.55921 factor:1 | 1 (-0.80189) | -1 | -1 |
| G: -5312.08863 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.79329 HOMO: -6.31848 LUMO: 1.67622 factor:1 | 1 (-0.33897) | -1 | -1 |
| G: -5312.08863 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.80742 HOMO: -6.50896 LUMO: 2.02725 factor:1 | 1 (-0.35309) | -1 | -1 |
| G: -5312.08863 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.01920 HOMO: -6.28583 LUMO: 2.00548 factor:1 | 1 (-0.56488) | -1 | -1 |
| G: -5312.08863 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.68891 HOMO: -6.67495 LUMO: 1.92384 factor:1 | 1 (-0.23459) | -1 | -1 |
| G: -5312.08863 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.49084 HOMO: -6.17154 LUMO: 2.39732 factor:1 | 1 (-0.03652) | -1 | -1 |
| G: -5312.08863 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.67669 HOMO: -6.84911 LUMO: 2.24766 factor:1 | 1 (-0.22237) | -1 | -1 |
| G: -5312.08863 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.59922 HOMO: -6.77564 LUMO: 2.38372 factor:1 | 1 (-0.14490) | -1 | -1 |
| G: -5312.08863 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.93433 HOMO: -6.18243 LUMO: 2.40821 factor:1 | 1 (-0.48001) | -1 | -1 |
| G: -5312.08863 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.64290 HOMO: -6.40828 LUMO: 2.22589 factor:1 | 1 (-0.18857) | -1 | -1 |
| G: -5312.08863 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.13787 HOMO: -6.74570 LUMO: 1.88303 factor:1 | 1 (-0.68355) | -1 | -1 |
| G: -5312.08863 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.85610 HOMO: -6.29944 LUMO: 2.05174 factor:1 | 1 (-0.40178) | -1 | -1 |
| G: -5312.08863 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.02211 HOMO: -7.00693 LUMO: 2.16331 factor:1 | 1 (-0.56779) | -1 | -1 |
| G: -5312.08863 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.09765 HOMO: -6.89537 LUMO: 2.19596 factor:1 | 1 (-0.64333) | -1 | -1 |
| G: -5312.08863 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.72420 HOMO: -6.72665 LUMO: 2.03813 factor:1 | 1 (-0.26988) | -1 | -1 |
| G: -5312.08863 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.97920 HOMO: -6.69944 LUMO: 2.36467 factor:1 | 1 (-0.52488) | -1 | -1 |
| G: -5312.08863 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.78480 HOMO: -6.92802 LUMO: 1.72792 factor:1 | 1 (-0.33048) | -1 | -1 |
| G: -5312.08863 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.86992 HOMO: -6.12256 LUMO: 1.85310 factor:1 | 1 (-0.41560) | -1 | -1 |
| G: -5312.08863 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.14786 HOMO: -6.70489 LUMO: 2.20956 factor:1 | 1 (-0.69354) | -1 | -1 |
| G: -5312.08863 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.73572 HOMO: -6.94707 LUMO: 1.81500 factor:1 | 1 (-0.28139) | -1 | -1 |
| G: -5312.08863 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.45800 HOMO: -6.39468 LUMO: 1.79051 factor:1 | 1 (-0.00367) | -1 | -1 |
| G: -5312.08863 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.77854 HOMO: -6.69128 LUMO: 2.03813 factor:1 | 1 (-1.32421) | -1 | -1 |
| G: -5312.08863 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.95933 HOMO: -6.55250 LUMO: 2.00548 factor:1 | 1 (-1.50501) | -1 | -1 |
| G: -5312.08863 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.75620 HOMO: -6.24773 LUMO: 2.09256 factor:1 | 1 (-1.30187) | -1 | -1 |
| G: -5312.08863 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.81748 HOMO: -6.85727 LUMO: 1.70071 factor:1 | 1 (-1.36315) | -1 | -1 |
| G: -5312.08863 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.87786 HOMO: -6.71305 LUMO: 1.72520 factor:1 | 1 (-1.42354) | -1 | -1 |
| G: -5312.08863 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11578.09582 HOMO: -6.81101 LUMO: 2.15514 factor:1 | 1 (-1.64150) | -1 | -1 |
| G: -5312.08863 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11578.06219 HOMO: -6.93618 LUMO: 1.75513 factor:1 | 1 (-1.60787) | -1 | -1 |
| G: -5312.08863 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.79258 HOMO: -6.63686 LUMO: 2.09800 factor:1 | 1 (-1.33826) | -1 | -1 |
| G: -5312.08863 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.97930 HOMO: -6.98244 LUMO: 1.72520 factor:1 | 1 (-1.52498) | -1 | -1 |
| G: -5312.08863 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.65464 HOMO: -6.37019 LUMO: 2.35923 factor:1 | 1 (-1.20032) | -1 | -1 |
| G: -5312.08863 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.59236 HOMO: -6.55794 LUMO: 2.12521 factor:1 | 1 (-1.13803) | -1 | -1 |
| G: -5312.08863 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.58583 HOMO: -6.45998 LUMO: 1.93201 factor:1 | 1 (-1.13150) | -1 | -1 |
| G: -5312.08863 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.70866 HOMO: -6.71033 LUMO: 1.58370 factor:1 | 1 (-1.25434) | -1 | -1 |
| G: -5312.08863 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.61007 HOMO: -6.67223 LUMO: 1.52928 factor:1 | 1 (-1.15575) | -1 | -1 |
| G: -5312.08863 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.45736 HOMO: -6.72121 LUMO: 1.33608 factor:1 | 1 (-1.00304) | -1 | -1 |
| G: -5312.08863 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.84159 HOMO: -6.89264 LUMO: 2.08983 factor:1 | 1 (-1.38726) | -1 | -1 |
| G: -5312.08863 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.73775 HOMO: -6.31032 LUMO: 2.24766 factor:1 | 1 (-1.28343) | -1 | -1 |
| G: -5312.08863 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.76866 HOMO: -6.79740 LUMO: 2.09528 factor:1 | 1 (-1.31434) | -1 | -1 |
| G: -5312.08863 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.69198 HOMO: -6.78108 LUMO: 2.15786 factor:1 | 1 (-1.23766) | -1 | -1 |
| G: -5312.08863 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.64398 HOMO: -6.50896 LUMO: 2.15786 factor:1 | 1 (-1.18965) | -1 | -1 |
| G: -5312.08863 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.45382 HOMO: -6.56067 LUMO: 2.24494 factor:1 | 1 (-0.99950) | -1 | -1 |
| G: -5312.08863 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.45067 HOMO: -6.72938 LUMO: 2.24494 factor:1 | 1 (-0.99634) | -1 | -1 |
| G: -5312.08863 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.73813 HOMO: -6.40556 LUMO: 1.58642 factor:1 | 1 (-1.28381) | -1 | -1 |
| G: -5312.08863 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.61706 HOMO: -6.63141 LUMO: 1.66262 factor:1 | 1 (-1.16274) | -1 | -1 |
| G: -5312.08863 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.77612 HOMO: -6.97156 LUMO: 2.23678 factor:1 | 1 (-1.32179) | -1 | -1 |
| G: -5312.08863 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.90036 HOMO: -6.86271 LUMO: 1.91296 factor:1 | 1 (-1.44604) | -1 | -1 |
| G: -5312.08863 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.63804 HOMO: -6.50624 LUMO: 1.89119 factor:1 | 1 (-1.18372) | -1 | -1 |
| G: -5312.08863 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.69415 HOMO: -6.70761 LUMO: 1.56193 factor:1 | 1 (-1.23983) | -1 | -1 |
| G: -5312.08863 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.90746 HOMO: -6.60420 LUMO: 1.79595 factor:1 | 1 (-1.45314) | -1 | -1 |
| G: -5312.08863 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.72390 HOMO: -6.85727 LUMO: 2.26943 factor:1 | 1 (-1.26957) | -1 | -1 |
| G: -5312.08863 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.56887 HOMO: -6.23413 LUMO: 1.91024 factor:1 | 1 (-1.11455) | -1 | -1 |
| G: -5312.08863 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.67791 HOMO: -6.84366 LUMO: 2.01364 factor:1 | 1 (-1.22359) | -1 | -1 |
| G: -5312.08863 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.82305 HOMO: -6.63414 LUMO: 2.54971 factor:1 | 1 (-1.36873) | -1 | -1 |
| G: -5312.08863 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.67788 HOMO: -6.52257 LUMO: 2.42998 factor:1 | 1 (-1.22356) | -1 | -1 |
| G: -5312.08863 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.51148 HOMO: -6.61509 LUMO: 2.31297 factor:1 | 1 (-1.05716) | -1 | -1 |
| G: -5312.08863 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.85220 HOMO: -6.45998 LUMO: 2.23405 factor:1 | 1 (-1.39788) | -1 | -1 |
| G: -5312.08863 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.90191 HOMO: -6.86271 LUMO: 2.22317 factor:1 | 1 (-1.44759) | -1 | -1 |
| G: -5312.08863 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.75690 HOMO: -6.84366 LUMO: 2.11432 factor:1 | 1 (-1.30258) | -1 | -1 |
| G: -5312.08863 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.96763 HOMO: -6.85999 LUMO: 2.44902 factor:1 | 1 (-1.51331) | -1 | -1 |
| G: -5312.08863 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.71554 HOMO: -6.73482 LUMO: 1.93745 factor:1 | 1 (-1.26122) | -1 | -1 |
| G: -5312.08863 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.29466 HOMO: -6.91441 LUMO: 2.32385 factor:1 | 1 (-0.84034) | -1 | -1 |
| G: -5312.08863 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.44297 HOMO: -6.16066 LUMO: 2.26399 factor:1 | 1 (-0.98864) | -1 | -1 |
| G: -5312.08863 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.58400 HOMO: -6.71305 LUMO: 2.38644 factor:1 | 1 (-1.12968) | -1 | -1 |
| G: -5312.08863 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.84418 HOMO: -7.08312 LUMO: 2.01636 factor:1 | 1 (-0.38986) | 1 | 1 |
| G: -5312.08863 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.94143 HOMO: -6.15249 LUMO: 1.90752 factor:1 | 1 (-0.48711) | -1 | -1 |
| G: -5312.08863 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.01006 HOMO: -6.83006 LUMO: 2.25855 factor:1 | 1 (-0.55574) | -1 | -1 |
| G: -5312.08863 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.90769 HOMO: -6.77836 LUMO: 2.24766 factor:1 | 1 (-0.45337) | -1 | -1 |
| G: -5312.08863 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.05496 HOMO: -6.66951 LUMO: 2.35923 factor:1 | 1 (-0.60064) | -1 | -1 |
| G: -5312.08863 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.99221 HOMO: -6.68312 LUMO: 2.30208 factor:1 | 1 (-0.53789) | -1 | -1 |
| G: -5312.08863 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.17472 HOMO: -6.49808 LUMO: 2.49801 factor:1 | 1 (-0.72039) | -1 | -1 |
| G: -5312.08863 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.13744 HOMO: -6.62325 LUMO: 1.89935 factor:1 | 1 (-0.68311) | -1 | -1 |
| G: -5312.08863 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.99251 HOMO: -6.80829 LUMO: 1.91296 factor:1 | 1 (-0.53819) | -1 | -1 |
| G: -5312.08863 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.84116 HOMO: -6.64230 LUMO: 2.13065 factor:1 | 1 (-0.38684) | -1 | -1 |
| G: -5312.08863 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.16936 HOMO: -6.40556 LUMO: 1.83949 factor:1 | 1 (-0.71503) | -1 | -1 |
| G: -5312.08863 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.78358 HOMO: -6.48175 LUMO: 1.72248 factor:1 | 1 (-0.32926) | -1 | -1 |
| G: -5312.08863 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.80780 HOMO: -6.61781 LUMO: 2.11432 factor:1 | 1 (-0.35348) | -1 | -1 |
| G: -5312.08863 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.70978 HOMO: -6.34570 LUMO: 2.22317 factor:1 | 1 (-0.25546) | -1 | -1 |
| G: -5312.08863 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.79713 HOMO: -7.00149 LUMO: 1.80139 factor:1 | 1 (-0.34281) | -1 | -1 |
| G: -5312.08863 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.78929 HOMO: -6.66951 LUMO: 2.13065 factor:1 | 1 (-0.33497) | -1 | -1 |
| G: -5312.08863 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.94217 HOMO: -6.54434 LUMO: 2.20140 factor:1 | 1 (-0.48785) | -1 | -1 |
| G: -5312.08863 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.12008 HOMO: -6.67767 LUMO: 2.02997 factor:1 | 1 (-0.66575) | -1 | -1 |
| G: -5312.08863 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.01882 HOMO: -6.49536 LUMO: 2.42998 factor:1 | 1 (-0.56450) | -1 | -1 |
| G: -5312.08863 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.95409 HOMO: -6.70761 LUMO: 2.71025 factor:1 | 1 (-0.49976) | -1 | -1 |
| G: -5312.08863 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.79112 HOMO: -6.62869 LUMO: 2.11160 factor:1 | 1 (-0.33680) | -1 | -1 |
| G: -5312.08863 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.77260 HOMO: -6.61781 LUMO: 2.24494 factor:1 | 1 (-1.31828) | -1 | -1 |
| G: -5312.08863 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.95446 HOMO: -6.66135 LUMO: 2.20956 factor:1 | 1 (-1.50014) | -1 | -1 |
| G: -5312.08863 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.84308 HOMO: -6.95523 LUMO: 2.03813 factor:1 | 1 (-1.38876) | -1 | -1 |
| G: -5312.08863 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.64814 HOMO: -7.11578 LUMO: 2.41365 factor:1 | 1 (-1.19382) | 1 | 1 |
| G: -5312.08863 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.96434 HOMO: -6.99061 LUMO: 2.13881 factor:1 | 1 (-1.51001) | -1 | -1 |
| G: -5312.08863 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.87887 HOMO: -6.43277 LUMO: 2.01364 factor:1 | 1 (-1.42454) | -1 | -1 |
| G: -5312.08863 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11578.05479 HOMO: -6.79196 LUMO: 2.04358 factor:1 | 1 (-1.60046) | -1 | -1 |
| G: -5312.08863 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.74382 HOMO: -7.08584 LUMO: 1.99732 factor:1 | 1 (-1.28949) | 1 | 1 |
| G: -5312.08863 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.70240 HOMO: -6.46815 LUMO: 2.29936 factor:1 | 1 (-1.24808) | -1 | -1 |
| G: -5312.08863 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11578.05517 HOMO: -6.78108 LUMO: 1.93745 factor:1 | 1 (-1.60085) | -1 | -1 |
| G: -5312.08863 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.78167 HOMO: -6.43277 LUMO: 1.80956 factor:1 | 1 (-1.32734) | -1 | -1 |
| G: -5312.08863 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.89421 HOMO: -6.71577 LUMO: -0.81090 factor:1 | 1 (-1.43989) | -1 | -1 |
| G: -5312.08863 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.70341 HOMO: -7.14027 LUMO: -0.68028 factor:1 | 1 (-1.24908) | -1 | -1 |
| G: -5312.08863 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.61546 HOMO: -7.03414 LUMO: -0.69661 factor:1 | 1 (-1.16114) | -1 | -1 |
| G: -5312.08863 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.47061 HOMO: -6.64502 LUMO: -0.47348 factor:1 | 1 (-1.01629) | -1 | -1 |
| G: -5312.08863 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.86670 HOMO: -6.60692 LUMO: 2.12793 factor:1 | 1 (-1.41238) | -1 | -1 |
| G: -5312.08863 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.66833 HOMO: -6.66407 LUMO: 1.94561 factor:1 | 1 (-1.21401) | -1 | -1 |
| G: -5312.08863 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.47921 HOMO: -7.10217 LUMO: 1.92384 factor:1 | 1 (-1.02489) | 1 | 1 |
| G: -5312.08863 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.68082 HOMO: -6.84094 LUMO: 1.66534 factor:1 | 1 (-1.22650) | -1 | -1 |
| G: -5312.08863 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.72773 HOMO: -6.93618 LUMO: 2.13065 factor:1 | 1 (-1.27341) | -1 | -1 |
| G: -5312.08863 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.64346 HOMO: -6.60692 LUMO: 2.20684 factor:1 | 1 (-1.18914) | -1 | -1 |
| G: -5312.08863 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.81846 HOMO: -6.85727 LUMO: 2.19324 factor:1 | 1 (-1.36413) | -1 | -1 |
| G: -5312.08863 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.85870 HOMO: -6.31032 LUMO: 1.76330 factor:1 | 1 (-1.40438) | -1 | -1 |
| G: -5312.08863 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.66534 HOMO: -6.43821 LUMO: 2.10072 factor:1 | 1 (-1.21102) | -1 | -1 |
| G: -5312.08863 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.54071 HOMO: -6.42189 LUMO: 2.19596 factor:1 | 1 (-1.08639) | -1 | -1 |
| G: -5312.08863 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.36441 HOMO: -6.40556 LUMO: 2.02181 factor:1 | 1 (-0.91008) | -1 | -1 |
| G: -5312.08863 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.77329 HOMO: -6.41372 LUMO: 2.26671 factor:1 | 1 (-1.31896) | -1 | -1 |
| G: -5312.08863 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.58389 HOMO: -6.60692 LUMO: 2.09800 factor:1 | 1 (-1.12957) | -1 | -1 |
| G: -5312.08863 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.74156 HOMO: -6.75931 LUMO: 1.76602 factor:1 | 1 (-1.28723) | -1 | -1 |
| G: -5312.08863 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.42620 HOMO: -6.39195 LUMO: 1.84221 factor:1 | 1 (-0.97188) | -1 | -1 |
| G: -5312.08863 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.33679 HOMO: -6.74570 LUMO: 2.04085 factor:1 | 1 (-0.88247) | -1 | -1 |
| G: -5312.08863 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.57853 HOMO: -6.77019 LUMO: 2.16875 factor:1 | 1 (-1.12421) | -1 | -1 |
| G: -5312.08863 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.45037 HOMO: -6.15522 LUMO: 1.81772 factor:1 | 1 (-0.99605) | -1 | -1 |
| G: -5312.08863 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.77092 HOMO: -6.48175 LUMO: 2.02453 factor:1 | 1 (-1.31660) | -1 | -1 |
| G: -5312.08863 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.41891 HOMO: -6.57427 LUMO: 1.77962 factor:1 | 1 (-0.96459) | -1 | -1 |
| G: -5312.08863 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.15923 HOMO: -6.57699 LUMO: 2.42998 factor:1 | 1 (-0.70491) | -1 | -1 |
| G: -5312.08863 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.44599 HOMO: -6.35386 LUMO: 2.25310 factor:1 | 1 (-0.99166) | -1 | -1 |
| G: -5312.08863 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.71337 HOMO: -6.80013 LUMO: 2.11160 factor:1 | 1 (-1.25904) | -1 | -1 |
| G: -5312.08863 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.48161 HOMO: -6.24229 LUMO: 2.05718 factor:1 | 1 (-1.02728) | -1 | -1 |
| G: -5312.08863 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.53709 HOMO: -6.42733 LUMO: 1.76874 factor:1 | 1 (-1.08277) | -1 | -1 |
| G: -5312.08863 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.56223 HOMO: -6.56883 LUMO: 2.36195 factor:1 | 1 (-1.10791) | -1 | -1 |
| G: -5312.08863 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.74335 HOMO: -6.72665 LUMO: 2.28848 factor:1 | 1 (-1.28903) | -1 | -1 |
| G: -5312.08863 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.69473 HOMO: -6.39195 LUMO: 1.79051 factor:1 | 1 (-1.24040) | -1 | -1 |
| G: -5312.08863 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.60112 HOMO: -6.70761 LUMO: 0.15510 factor:1 | 1 (-1.14680) | -1 | -1 |
| G: -5312.08863 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.88172 HOMO: -6.44366 LUMO: -0.16871 factor:1 | 1 (-1.42740) | -1 | -1 |
| G: -5312.08863 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.58727 HOMO: -6.68584 LUMO: 1.69527 factor:1 | 1 (-1.13295) | -1 | -1 |
| G: -5312.08863 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.75617 HOMO: -6.26950 LUMO: 1.61636 factor:1 | 1 (-1.30185) | -1 | -1 |
| G: -5312.08863 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.61453 HOMO: -6.47631 LUMO: 1.98915 factor:1 | 1 (-1.16021) | -1 | -1 |
| G: -5312.08863 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.53644 HOMO: -6.58243 LUMO: 1.97283 factor:1 | 1 (-1.08212) | -1 | -1 |
| G: -5312.08863 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.42729 HOMO: -6.51713 LUMO: 1.97283 factor:1 | 1 (-0.97297) | -1 | -1 |
| G: -5312.08863 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.44610 HOMO: -6.65046 LUMO: 1.69255 factor:1 | 1 (-0.99177) | -1 | -1 |
| G: -5312.08863 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.71035 HOMO: -6.26406 LUMO: 2.21773 factor:1 | 1 (-1.25602) | -1 | -1 |
| G: -5312.08863 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.81843 HOMO: -6.88992 LUMO: 2.28304 factor:1 | 1 (-1.36411) | -1 | -1 |
| G: -5312.08863 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.60485 HOMO: -6.67767 LUMO: 2.34834 factor:1 | 1 (-1.15052) | -1 | -1 |
| G: -5312.08863 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.39369 HOMO: -6.52801 LUMO: 2.10344 factor:1 | 1 (-0.93936) | -1 | -1 |
| G: -5312.08863 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.43410 HOMO: -6.52801 LUMO: 2.24222 factor:1 | 1 (-0.97977) | -1 | -1 |
| G: -5312.08863 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.32702 HOMO: -6.17154 LUMO: 1.89663 factor:1 | 1 (-0.87270) | -1 | -1 |
| G: -5312.08863 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.18974 HOMO: -6.42733 LUMO: 2.15514 factor:1 | 1 (-0.73541) | -1 | -1 |
| G: -5312.08863 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.70643 HOMO: -6.36474 LUMO: 2.01364 factor:1 | 1 (-1.25210) | -1 | -1 |
| G: -5312.08863 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.48514 HOMO: -6.82189 LUMO: 1.86942 factor:1 | 1 (-1.03082) | -1 | -1 |
| G: -5312.08863 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.14612 HOMO: -6.60148 LUMO: 2.00548 factor:1 | 1 (-0.69180) | -1 | -1 |
| G: -5312.08863 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.21548 HOMO: -6.67767 LUMO: 2.15786 factor:1 | 1 (-0.76116) | -1 | -1 |
| G: -5312.08863 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.52841 HOMO: -6.79196 LUMO: 2.06534 factor:1 | 1 (-1.07409) | -1 | -1 |
| G: -5312.08863 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.30457 HOMO: -6.70216 LUMO: 1.83405 factor:1 | 1 (-0.85025) | -1 | -1 |
| G: -5312.08863 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.37135 HOMO: -6.58788 LUMO: 1.79051 factor:1 | 1 (-0.91702) | -1 | -1 |
| G: -5312.08863 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11578.10940 HOMO: -6.34842 LUMO: 1.80139 factor:1 | 1 (-1.65508) | -1 | -1 |
| G: -5312.08863 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11578.39055 HOMO: -6.48175 LUMO: 1.95922 factor:1 | 1 (-1.93623) | -1 | -1 |
| G: -5312.08863 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11578.98925 HOMO: -6.71033 LUMO: 2.02997 factor:1 | 1 (-2.53493) | -1 | -1 |
| G: -5312.08863 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.70591 HOMO: -6.89264 LUMO: 2.42726 factor:1 | 1 (-1.25159) | -1 | -1 |
| G: -5312.08863 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11578.13473 HOMO: -6.74570 LUMO: 2.20684 factor:1 | 1 (-1.68041) | -1 | -1 |
| G: -5312.08863 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.74743 HOMO: -6.30216 LUMO: 2.15242 factor:1 | 1 (-1.29311) | -1 | -1 |
| G: -5312.08863 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11578.17299 HOMO: -6.94979 LUMO: 2.43814 factor:1 | 1 (-1.71867) | -1 | -1 |
| G: -5312.08863 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.99476 HOMO: -6.97972 LUMO: 2.11432 factor:1 | 1 (-1.54044) | -1 | -1 |
| G: -5312.08863 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11578.38946 HOMO: -6.17154 LUMO: 1.98099 factor:1 | 1 (-1.93514) | -1 | -1 |
| G: -5312.08863 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11578.93761 HOMO: -6.74026 LUMO: 2.21501 factor:1 | 1 (-2.48328) | -1 | -1 |
| G: -5312.08863 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11578.19879 HOMO: -6.72393 LUMO: 2.19596 factor:1 | 1 (-1.74447) | -1 | -1 |
| G: -5312.08863 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11578.45123 HOMO: -6.11440 LUMO: 2.10072 factor:1 | 1 (-1.99691) | -1 | -1 |
| G: -5312.08863 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11579.10898 HOMO: -6.34297 LUMO: 1.92657 factor:1 | 1 (-2.65466) | -1 | -1 |
| G: -5312.08863 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11578.98863 HOMO: -6.24773 LUMO: 2.00276 factor:1 | 1 (-2.53431) | -1 | -1 |
| G: -5312.08863 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.81339 HOMO: -6.75114 LUMO: 1.98643 factor:1 | 1 (-1.35907) | -1 | -1 |
| G: -5312.08863 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.96306 HOMO: -6.69128 LUMO: 2.08711 factor:1 | 1 (-1.50874) | -1 | -1 |
| G: -5312.08863 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11578.29947 HOMO: -6.65318 LUMO: 2.15514 factor:1 | 1 (-1.84515) | -1 | -1 |
| G: -5312.08863 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11578.18761 HOMO: -6.67495 LUMO: 1.72248 factor:1 | 1 (-1.73328) | -1 | -1 |
| G: -5312.08863 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.91223 HOMO: -6.58243 LUMO: 1.83405 factor:1 | 1 (-1.45790) | -1 | -1 |
| G: -5312.08863 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.69005 HOMO: -6.61237 LUMO: 1.69799 factor:1 | 1 (-0.23573) | -1 | -1 |
| G: -5312.08863 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.85564 HOMO: -6.57427 LUMO: 2.29936 factor:1 | 1 (-0.40131) | -1 | -1 |
| G: -5312.08863 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.10307 HOMO: -6.40012 LUMO: 2.35378 factor:1 | 1 (-0.64875) | -1 | -1 |
| G: -5312.08863 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.79169 HOMO: -6.90081 LUMO: 2.26671 factor:1 | 1 (-0.33737) | -1 | -1 |
| G: -5312.08863 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.60589 HOMO: -6.44910 LUMO: 2.25855 factor:1 | 1 (-0.15157) | -1 | -1 |
| G: -5312.08863 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.64028 HOMO: -6.61509 LUMO: 2.26943 factor:1 | 1 (-0.18596) | -1 | -1 |
| G: -5312.08863 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.65004 HOMO: -6.78924 LUMO: 2.09256 factor:1 | 1 (-1.19572) | -1 | -1 |
| G: -5312.08863 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11578.51580 HOMO: -6.47087 LUMO: 1.97555 factor:1 | 1 (-2.06148) | -1 | -1 |
| G: -5312.08863 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.97723 HOMO: -6.75931 LUMO: 1.98643 factor:1 | 1 (-1.52291) | -1 | -1 |
| G: -5312.08863 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.83108 HOMO: -6.17971 LUMO: 2.09800 factor:1 | 1 (-1.37676) | -1 | -1 |
| G: -5312.08863 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.58085 HOMO: -6.83006 LUMO: 1.91840 factor:1 | 1 (-1.12652) | -1 | -1 |
| G: -5312.08863 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.70308 HOMO: -6.72938 LUMO: 2.17419 factor:1 | 1 (-1.24876) | -1 | -1 |
| G: -5312.08863 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.59279 HOMO: -6.78924 LUMO: 2.42726 factor:1 | 1 (-1.13847) | -1 | -1 |
| G: -5312.08863 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.80050 HOMO: -6.41372 LUMO: 1.93745 factor:1 | 1 (-1.34617) | -1 | -1 |
| G: -5312.08863 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.65772 HOMO: -6.85455 LUMO: 2.14970 factor:1 | 1 (-1.20340) | -1 | -1 |
| G: -5312.08863 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.96877 HOMO: -6.38651 LUMO: 2.18507 factor:1 | 1 (-1.51445) | -1 | -1 |
| G: -5312.08863 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.76395 HOMO: -6.81373 LUMO: 2.00548 factor:1 | 1 (-1.30963) | -1 | -1 |
| G: -5312.08863 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11578.12815 HOMO: -6.64774 LUMO: 2.41365 factor:1 | 1 (-1.67383) | -1 | -1 |
| G: -5312.08863 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.97669 HOMO: -6.70489 LUMO: 2.31569 factor:1 | 1 (-1.52237) | -1 | -1 |
| G: -5312.08863 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11578.22407 HOMO: -6.49264 LUMO: 1.78779 factor:1 | 1 (-1.76975) | -1 | -1 |
| G: -5312.08863 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11578.80087 HOMO: -6.81101 LUMO: 1.86670 factor:1 | 1 (-2.34655) | -1 | -1 |
| G: -5312.08863 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11578.38970 HOMO: -6.72121 LUMO: 1.48846 factor:1 | 1 (-1.93538) | -1 | -1 |
| G: -5312.08863 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11578.15218 HOMO: -6.35930 LUMO: 1.78507 factor:1 | 1 (-1.69785) | -1 | -1 |
| G: -5312.08863 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.71168 HOMO: -6.38651 LUMO: 2.04358 factor:1 | 1 (-1.25736) | -1 | -1 |
| G: -5312.08863 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.95879 HOMO: -6.42189 LUMO: 1.99187 factor:1 | 1 (-1.50446) | -1 | -1 |
| G: -5312.08863 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.95217 HOMO: -6.69400 LUMO: 1.61091 factor:1 | 1 (-1.49785) | -1 | -1 |
| G: -5312.08863 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.82006 HOMO: -6.81101 LUMO: 2.17419 factor:1 | 1 (-1.36574) | -1 | -1 |
| G: -5312.08863 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.56789 HOMO: -6.90897 LUMO: 2.28576 factor:1 | 1 (-1.11357) | -1 | -1 |
| G: -5312.08863 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.91496 HOMO: -6.75387 LUMO: 2.31297 factor:1 | 1 (-0.46063) | -1 | -1 |
| G: -5312.08863 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.82407 HOMO: -7.05863 LUMO: 2.18780 factor:1 | 1 (-0.36975) | -1 | -1 |
| G: -5312.08863 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.93324 HOMO: -6.56611 LUMO: 1.99187 factor:1 | 1 (-0.47892) | -1 | -1 |
| G: -5312.08863 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.17480 HOMO: -6.59060 LUMO: 1.86398 factor:1 | 1 (-0.72048) | -1 | -1 |
| G: -5312.08863 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.12565 HOMO: -6.59060 LUMO: 1.59459 factor:1 | 1 (-0.67133) | -1 | -1 |
| G: -5312.08863 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.96225 HOMO: -6.57699 LUMO: 1.48030 factor:1 | 1 (-0.50793) | -1 | -1 |
| G: -5312.08863 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.93771 HOMO: -6.99605 LUMO: 2.30208 factor:1 | 1 (-0.48338) | -1 | -1 |
| G: -5312.08863 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.74475 HOMO: -6.42189 LUMO: 2.20412 factor:1 | 1 (-0.29043) | -1 | -1 |
| G: -5312.08863 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.76276 HOMO: -7.15115 LUMO: 1.83405 factor:1 | 1 (-0.30844) | 1 | 1 |
| G: -5312.08863 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.68878 HOMO: -7.08040 LUMO: 2.21773 factor:1 | 1 (-0.23445) | 1 | 1 |
| G: -5312.08863 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.82366 HOMO: -6.72121 LUMO: 1.89663 factor:1 | 1 (-0.36934) | -1 | -1 |
| G: -5312.08863 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.95049 HOMO: -6.25590 LUMO: 1.85037 factor:1 | 1 (-0.49617) | -1 | -1 |
| G: -5312.08863 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.92440 HOMO: -6.70489 LUMO: 1.98915 factor:1 | 1 (-0.47008) | -1 | -1 |
| G: -5312.08863 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.05412 HOMO: -6.53617 LUMO: 2.08439 factor:1 | 1 (-0.59979) | -1 | -1 |
| G: -5312.08863 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.09031 HOMO: -6.69944 LUMO: 1.98915 factor:1 | 1 (-0.63598) | -1 | -1 |
| G: -5312.08863 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.87694 HOMO: -6.79468 LUMO: 1.96466 factor:1 | 1 (-0.42262) | -1 | -1 |
| G: -5312.08863 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.82834 HOMO: -6.79468 LUMO: 1.99459 factor:1 | 1 (-0.37402) | -1 | -1 |
| G: -5312.08863 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.66026 HOMO: -6.58788 LUMO: 1.98371 factor:1 | 1 (-0.20594) | -1 | -1 |
| G: -5312.08863 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.80815 HOMO: -6.58788 LUMO: 2.16603 factor:1 | 1 (-0.35383) | -1 | -1 |
| G: -5312.08863 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.68761 HOMO: -6.56883 LUMO: 1.64085 factor:1 | 1 (-0.23328) | -1 | -1 |
| G: -5312.08863 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.85621 HOMO: -7.19197 LUMO: 2.66127 factor:1 | 1 (-0.40188) | 1 | 1 |
| G: -5312.08863 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.69539 HOMO: -6.48175 LUMO: 2.40004 factor:1 | 1 (-0.24107) | -1 | -1 |
| G: -5312.08863 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.11999 HOMO: -6.18515 LUMO: 2.27759 factor:1 | 1 (-0.66567) | -1 | -1 |
| G: -5312.08863 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.89506 HOMO: -6.64774 LUMO: 2.13337 factor:1 | 1 (-0.44074) | -1 | -1 |
| G: -5312.08863 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.90440 HOMO: -6.39740 LUMO: 1.95106 factor:1 | 1 (-0.45008) | -1 | -1 |
| G: -5312.08863 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.75476 HOMO: -6.59332 LUMO: 1.81772 factor:1 | 1 (-0.30044) | -1 | -1 |
| G: -5312.08863 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.67280 HOMO: -6.68312 LUMO: 2.41909 factor:1 | 1 (-0.21848) | -1 | -1 |
| G: -5312.08863 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.55190 HOMO: -5.87494 LUMO: 2.18235 factor:1 | 1 (-0.09758) | -1 | -1 |
| G: -5312.08863 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.70110 HOMO: -6.30488 LUMO: 2.04902 factor:1 | 1 (-0.24678) | -1 | -1 |
| G: -5312.08863 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.94277 HOMO: -6.65046 LUMO: 2.05446 factor:1 | 1 (-0.48844) | -1 | -1 |
| G: -5312.08863 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11578.14483 HOMO: -6.55794 LUMO: 2.06807 factor:1 | 1 (-1.69051) | -1 | -1 |
| G: -5312.08863 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11579.07984 HOMO: -6.68040 LUMO: 1.99187 factor:1 | 1 (-2.62552) | -1 | -1 |
| G: -5312.08863 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11578.29335 HOMO: -6.60965 LUMO: 2.18780 factor:1 | 1 (-1.83903) | -1 | -1 |
| G: -5312.08863 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11578.20937 HOMO: -6.88176 LUMO: 2.10344 factor:1 | 1 (-1.75505) | -1 | -1 |
| G: -5312.08863 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.98635 HOMO: -6.63414 LUMO: 1.70615 factor:1 | 1 (-1.53203) | -1 | -1 |
| G: -5312.08863 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.75493 HOMO: -7.15115 LUMO: 2.07351 factor:1 | 1 (-0.30060) | 1 | 1 |
| G: -5312.08863 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.73351 HOMO: -6.85727 LUMO: 2.27759 factor:1 | 1 (-0.27919) | -1 | -1 |
| G: -5312.08863 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.96571 HOMO: -6.91713 LUMO: 2.28848 factor:1 | 1 (-0.51138) | -1 | -1 |
| G: -5312.08863 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.84187 HOMO: -7.10217 LUMO: 2.14698 factor:1 | 1 (-0.38754) | 1 | 1 |
| G: -5312.08863 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.59903 HOMO: -6.78108 LUMO: 2.45447 factor:1 | 1 (-0.14471) | -1 | -1 |
| G: -5312.08863 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.50972 HOMO: -6.78380 LUMO: 2.43542 factor:1 | 1 (-0.05540) | -1 | -1 |
| G: -5312.08863 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.69416 HOMO: -6.60965 LUMO: 2.33474 factor:1 | 1 (-0.23984) | -1 | -1 |
| G: -5312.08863 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.87185 HOMO: -6.72665 LUMO: 2.25855 factor:1 | 1 (-0.41753) | -1 | -1 |
| G: -5312.08863 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.73758 HOMO: -6.27495 LUMO: 2.04358 factor:1 | 1 (-1.28326) | -1 | -1 |
| G: -5312.08863 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11578.44568 HOMO: -6.17426 LUMO: 1.45853 factor:1 | 1 (-1.99136) | -1 | -1 |
| G: -5312.08863 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.76953 HOMO: -7.21374 LUMO: 2.33474 factor:1 | 1 (-1.31521) | 1 | 1 |
| G: -5312.08863 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.97966 HOMO: -6.94707 LUMO: 1.81772 factor:1 | 1 (-1.52533) | -1 | -1 |
| G: -5312.08863 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.87266 HOMO: -6.80829 LUMO: 0.17960 factor:1 | 1 (-1.41834) | -1 | -1 |
| G: -5312.08863 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.59456 HOMO: -7.19469 LUMO: 1.60819 factor:1 | 1 (-1.14024) | 1 | 1 |
| G: -5312.08863 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.75707 HOMO: -6.78652 LUMO: 0.53334 factor:1 | 1 (-1.30275) | -1 | -1 |
| G: -5312.08863 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.92602 HOMO: -6.70489 LUMO: 0.74559 factor:1 | 1 (-1.47170) | -1 | -1 |
| G: -5312.08863 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.78575 HOMO: -6.72393 LUMO: 0.88981 factor:1 | 1 (-1.33143) | -1 | -1 |
| G: -5312.08863 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.54844 HOMO: -4.54430 LUMO: -0.90614 factor:1 | 1 (-1.09412) | -1 | -1 |
| G: -5312.08863 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11578.10545 HOMO: -6.83006 LUMO: 0.47348 factor:1 | 1 (-1.65113) | -1 | -1 |
| G: -5312.08863 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.93704 HOMO: -7.07496 LUMO: 0.50613 factor:1 | 1 (-1.48272) | -1 | -1 |
| G: -5312.08863 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11578.16984 HOMO: -6.62053 LUMO: 0.74559 factor:1 | 1 (-1.71551) | -1 | -1 |
| G: -5312.08863 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.91927 HOMO: -6.79196 LUMO: 1.80139 factor:1 | 1 (-1.46495) | -1 | -1 |
| G: -5312.08863 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11578.07949 HOMO: -6.71033 LUMO: 0.40817 factor:1 | 1 (-1.62517) | -1 | -1 |
| G: -5312.08863 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.76567 HOMO: -6.74026 LUMO: 0.95784 factor:1 | 1 (-0.31135) | -1 | -1 |
| G: -5312.08863 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.54853 HOMO: -7.34707 LUMO: 0.40001 factor:1 | 1 (-0.09421) | -1 | -1 |
| G: -5312.08863 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.85596 HOMO: -6.19875 LUMO: -0.88709 factor:1 | 1 (-0.40164) | -1 | -1 |
| G: -5312.08863 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.59808 HOMO: -6.48719 LUMO: -0.14694 factor:1 | 1 (-0.14376) | -1 | -1 |
| G: -5312.08863 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.81115 HOMO: -6.73482 LUMO: -0.01633 factor:1 | 1 (-0.35682) | -1 | -1 |
| G: -5312.08863 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.78461 HOMO: -7.05591 LUMO: -0.20136 factor:1 | 1 (-0.33029) | -1 | -1 |
| G: -5312.08863 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.56692 HOMO: -6.38651 LUMO: -2.07895 factor:1 | 1 (-0.11260) | -1 | -1 |
| G: -5312.08863 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.54436 HOMO: -6.85455 LUMO: -1.03403 factor:1 | 1 (-0.09004) | -1 | -1 |
| G: -5312.08863 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.34899 HOMO: -6.72121 LUMO: -0.99322 factor:1 | -1 (0.10534) | -1 | -1 |
| G: -5312.08863 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.72344 HOMO: -6.53890 LUMO: -0.10885 factor:1 | 1 (-0.26912) | -1 | -1 |
| G: -5312.08863 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.74235 HOMO: -6.68312 LUMO: 0.21225 factor:1 | 1 (-1.28802) | -1 | -1 |
| G: -5312.08863 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.55516 HOMO: -6.68040 LUMO: 0.21225 factor:1 | 1 (-1.10084) | -1 | -1 |
| G: -5312.08863 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11578.59292 HOMO: -6.76475 LUMO: -0.64491 factor:1 | 1 (-2.13860) | -1 | -1 |
| G: -5312.08863 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.58553 HOMO: -6.48175 LUMO: 0.41633 factor:1 | 1 (-1.13120) | -1 | -1 |
| G: -5312.08863 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.82621 HOMO: -6.42733 LUMO: 0.16599 factor:1 | 1 (-1.37189) | -1 | -1 |
| G: -5312.08863 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.78539 HOMO: -6.66679 LUMO: 0.77825 factor:1 | 1 (-1.33107) | -1 | -1 |
| G: -5312.08863 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.81100 HOMO: -6.75931 LUMO: -0.73471 factor:1 | 1 (-1.35668) | -1 | -1 |
| G: -5312.08863 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.61336 HOMO: -6.53617 LUMO: 0.38096 factor:1 | 1 (-1.15904) | -1 | -1 |
| G: -5312.08863 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.80537 HOMO: -6.34297 LUMO: 0.35375 factor:1 | 1 (-1.35105) | -1 | -1 |
| G: -5312.08863 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.02780 HOMO: -7.11850 LUMO: -0.03265 factor:1 | 1 (-0.57348) | -1 | -1 |
| G: -5312.08863 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.89789 HOMO: -5.21914 LUMO: 1.29798 factor:1 | 1 (-0.44357) | -1 | -1 |
| G: -5312.08863 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.94946 HOMO: -7.09129 LUMO: -0.66668 factor:1 | 1 (-0.49514) | -1 | -1 |
| G: -5312.08863 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.06759 HOMO: -6.96884 LUMO: -0.31021 factor:1 | 1 (-0.61326) | -1 | -1 |
| G: -5312.08863 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.90641 HOMO: -6.51713 LUMO: -0.59865 factor:1 | 1 (-0.45209) | -1 | -1 |
| G: -5312.08863 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.71041 HOMO: -6.69400 LUMO: -0.07075 factor:1 | 1 (-0.25609) | -1 | -1 |
| G: -5312.08863 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.81270 HOMO: -5.28173 LUMO: 1.17281 factor:1 | 1 (-0.35837) | -1 | -1 |
| G: -5312.08863 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.96054 HOMO: -6.54434 LUMO: 0.32109 factor:1 | 1 (-0.50621) | -1 | -1 |
| G: -5312.08863 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.21268 HOMO: -6.79740 LUMO: -0.24762 factor:1 | 1 (-0.75835) | -1 | -1 |
| G: -5312.08863 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.08187 HOMO: -6.91986 LUMO: -0.14694 factor:1 | 1 (-0.62755) | -1 | -1 |
| G: -5312.08863 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.20574 HOMO: -6.75114 LUMO: 0.18504 factor:1 | 1 (-0.75142) | -1 | -1 |
| G: -5312.08863 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.07199 HOMO: -6.74842 LUMO: 0.69389 factor:1 | 1 (-0.61767) | -1 | -1 |
| G: -5312.08863 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.04816 HOMO: -7.01782 LUMO: 0.56600 factor:1 | 1 (-0.59383) | -1 | -1 |
| G: -5312.08863 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.85226 HOMO: -6.47359 LUMO: -0.56600 factor:1 | 1 (-0.39794) | -1 | -1 |
| G: -5312.08863 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.98435 HOMO: -6.63686 LUMO: -0.55783 factor:1 | 1 (-0.53002) | -1 | -1 |
| G: -5312.08863 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.01730 HOMO: -4.13885 LUMO: -2.05446 factor:1 | 1 (-0.56298) | -1 | -1 |
| G: -5312.08863 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.18955 HOMO: -6.34570 LUMO: 0.19864 factor:1 | 1 (-0.73522) | -1 | -1 |
| G: -5312.08863 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.97814 HOMO: -6.47903 LUMO: 0.24762 factor:1 | 1 (-0.52382) | -1 | -1 |
| G: -5312.08863 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.21940 HOMO: -6.15249 LUMO: 0.32109 factor:1 | 1 (-0.76508) | -1 | -1 |
| G: -5312.08863 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.05120 HOMO: -6.84366 LUMO: 0.29116 factor:1 | 1 (-0.59688) | -1 | -1 |
| G: -5312.08863 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.80480 HOMO: -6.34297 LUMO: 0.19864 factor:1 | 1 (-0.35048) | -1 | -1 |
| G: -5312.08863 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.98315 HOMO: -6.51168 LUMO: 0.30749 factor:1 | 1 (-0.52883) | -1 | -1 |
| G: -5312.08863 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.86979 HOMO: -6.79468 LUMO: -0.16599 factor:1 | 1 (-0.41546) | -1 | -1 |
| G: -5312.08863 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.76970 HOMO: -7.24095 LUMO: 0.15238 factor:1 | 1 (-0.31538) | -1 | -1 |
| G: -5312.08863 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.98927 HOMO: -7.06952 LUMO: -0.34558 factor:1 | 1 (-0.53495) | -1 | -1 |
| G: -5312.08863 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.84516 HOMO: -6.88176 LUMO: 0.02177 factor:1 | 1 (-0.39084) | -1 | -1 |
| G: -5312.08863 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.12816 HOMO: -6.37291 LUMO: -0.69117 factor:1 | 1 (-0.67384) | -1 | -1 |
| G: -5312.08863 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.92805 HOMO: -6.83278 LUMO: -0.59049 factor:1 | 1 (-0.47372) | -1 | -1 |
| G: -5312.08863 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.12729 HOMO: -6.57155 LUMO: -0.33470 factor:1 | 1 (-0.67296) | -1 | -1 |
| G: -5312.08863 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.93028 HOMO: -6.89537 LUMO: -0.58504 factor:1 | 1 (-0.47595) | -1 | -1 |
| G: -5312.08863 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.77710 HOMO: -6.57155 LUMO: -0.34831 factor:1 | 1 (-0.32278) | -1 | -1 |
| G: -5312.08863 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.84151 HOMO: -6.64774 LUMO: -0.95784 factor:1 | 1 (-0.38719) | -1 | -1 |
| G: -5312.08863 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.59060 HOMO: -6.91713 LUMO: -0.69933 factor:1 | 1 (-0.13627) | -1 | -1 |
| G: -5312.08863 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.63027 HOMO: -6.80557 LUMO: -0.65035 factor:1 | 1 (-0.17595) | -1 | -1 |
| G: -5312.08863 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.60276 HOMO: -7.26544 LUMO: -0.79729 factor:1 | 1 (-0.14844) | -1 | -1 |
| G: -5312.08863 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.47770 HOMO: -6.69128 LUMO: -0.16871 factor:1 | 1 (-0.02337) | -1 | -1 |
| G: -5312.08863 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.97346 HOMO: -6.88448 LUMO: 0.13061 factor:1 | 1 (-0.51914) | -1 | -1 |
| G: -5312.08863 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.07588 HOMO: -6.50352 LUMO: 0.12245 factor:1 | 1 (-0.62156) | -1 | -1 |
| G: -5312.08863 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.02892 HOMO: -6.56067 LUMO: 0.17687 factor:1 | 1 (-0.57460) | -1 | -1 |
| G: -5312.08863 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.90965 HOMO: -6.70216 LUMO: 0.25034 factor:1 | 1 (-0.45533) | -1 | -1 |
| G: -5312.08863 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.13540 HOMO: -6.51713 LUMO: -0.78369 factor:1 | 1 (-0.68107) | -1 | -1 |
| G: -5312.08863 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.24680 HOMO: -6.50352 LUMO: 0.12245 factor:1 | 1 (-0.79248) | -1 | -1 |
| G: -5312.08863 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.13428 HOMO: -6.22052 LUMO: -0.83811 factor:1 | 1 (-0.67996) | -1 | -1 |
| G: -5312.08863 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.15844 HOMO: -6.51168 LUMO: -0.76464 factor:1 | 1 (-0.70412) | -1 | -1 |
| G: -5312.08863 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.02046 HOMO: -7.14571 LUMO: -0.80274 factor:1 | 1 (-0.56613) | -1 | -1 |
| G: -5312.08863 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.83944 HOMO: -6.66679 LUMO: -0.88709 factor:1 | 1 (-0.38512) | -1 | -1 |
| G: -5312.08863 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.77604 HOMO: -6.76203 LUMO: -1.43948 factor:1 | 1 (-0.32172) | -1 | -1 |
| G: -5312.08863 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.79210 HOMO: -6.57427 LUMO: -1.62996 factor:1 | 1 (-0.33777) | -1 | -1 |
| G: -5312.08863 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.98617 HOMO: -5.05043 LUMO: 1.24900 factor:1 | 1 (-0.53185) | -1 | -1 |
| G: -5312.08863 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.66085 HOMO: -6.53345 LUMO: 0.23130 factor:1 | 1 (-1.20653) | -1 | -1 |
| G: -5312.08863 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.42819 HOMO: -7.18381 LUMO: -0.22585 factor:1 | 1 (-0.97387) | -1 | -1 |
| G: -5312.08863 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.75987 HOMO: -7.00965 LUMO: -1.79595 factor:1 | 1 (-1.30555) | -1 | -1 |
| G: -5312.08863 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.91451 HOMO: -6.08174 LUMO: -0.82995 factor:1 | 1 (-1.46019) | -1 | -1 |
| G: -5312.08863 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.72196 HOMO: -6.42189 LUMO: -0.84355 factor:1 | 1 (-1.26764) | -1 | -1 |
| G: -5312.08863 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.96485 HOMO: -6.53890 LUMO: 0.60409 factor:1 | 1 (-1.51053) | -1 | -1 |
| G: -5312.08863 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.49037 HOMO: -6.62869 LUMO: 0.43810 factor:1 | 1 (-1.03605) | -1 | -1 |
| G: -5312.08863 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.46819 HOMO: -6.68312 LUMO: 0.64491 factor:1 | 1 (-1.01387) | -1 | -1 |
| G: -5312.08863 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.34155 HOMO: -6.42189 LUMO: 1.51295 factor:1 | 1 (-0.88723) | -1 | -1 |
| G: -5312.08863 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.64501 HOMO: -6.17971 LUMO: 1.67622 factor:1 | 1 (-1.19069) | -1 | -1 |
| G: -5312.08863 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.70632 HOMO: -6.79196 LUMO: 1.36873 factor:1 | 1 (-1.25200) | -1 | -1 |
| G: -5312.08863 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.79822 HOMO: -7.38517 LUMO: 0.56328 factor:1 | 1 (-0.34390) | 1 | 1 |
| G: -5312.08863 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.84396 HOMO: -7.56204 LUMO: 0.71566 factor:1 | 1 (-0.38964) | 1 | 1 |
| G: -5312.08863 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.08105 HOMO: -6.45726 LUMO: -1.91840 factor:1 | 1 (-0.62673) | -1 | -1 |
| G: -5312.08863 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.68439 HOMO: -6.13073 LUMO: -0.97417 factor:1 | 1 (-0.23007) | -1 | -1 |
| G: -5312.08863 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.87164 HOMO: -6.50352 LUMO: -0.69661 factor:1 | 1 (-0.41731) | -1 | -1 |
| G: -5312.08863 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.73591 HOMO: -6.76747 LUMO: -1.71976 factor:1 | 1 (-0.28158) | -1 | -1 |
| G: -5312.08863 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.89139 HOMO: -6.48447 LUMO: -0.89525 factor:1 | 1 (-0.43707) | -1 | -1 |
| G: -5312.08863 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.15583 HOMO: -7.11850 LUMO: -0.71566 factor:1 | 1 (-0.70151) | -1 | -1 |
| G: -5312.08863 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.85346 HOMO: -6.80285 LUMO: -0.49253 factor:1 | 1 (-0.39914) | -1 | -1 |
| G: -5312.08863 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.84862 HOMO: -6.80557 LUMO: -0.88165 factor:1 | 1 (-0.39429) | -1 | -1 |
| G: -5312.08863 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.71857 HOMO: -6.94162 LUMO: -0.08980 factor:1 | 1 (-0.26425) | -1 | -1 |
| G: -5312.08863 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.41503 HOMO: -6.97972 LUMO: -0.29388 factor:1 | -1 (0.03929) | -1 | -1 |
| G: -5312.08863 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.74089 HOMO: -6.75114 LUMO: 0.04626 factor:1 | 1 (-0.28656) | -1 | -1 |
| G: -5312.08863 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.96562 HOMO: -7.15932 LUMO: 0.68845 factor:1 | 1 (-0.51130) | 1 | 1 |
| G: -5312.08863 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.63555 HOMO: -7.36612 LUMO: 0.63675 factor:1 | 1 (-0.18123) | 1 | 1 |
| G: -5312.08863 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.75743 HOMO: -7.02598 LUMO: -0.66124 factor:1 | 1 (-0.30311) | -1 | -1 |
| G: -5312.08863 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.54842 HOMO: -6.89264 LUMO: -0.54967 factor:1 | 1 (-0.09410) | -1 | -1 |
| G: -5312.08863 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.11017 HOMO: -6.97700 LUMO: 0.27756 factor:1 | 1 (-0.65585) | -1 | -1 |
| G: -5312.08863 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.75640 HOMO: -6.60965 LUMO: 0.08163 factor:1 | 1 (-0.30207) | -1 | -1 |
| G: -5312.08863 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.62377 HOMO: -6.70761 LUMO: 0.40001 factor:1 | 1 (-0.16945) | -1 | -1 |
| G: -5312.08863 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.77509 HOMO: -6.69128 LUMO: 0.23674 factor:1 | 1 (-0.32077) | -1 | -1 |
| G: -5312.08863 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.97354 HOMO: -6.69128 LUMO: -0.69933 factor:1 | 1 (-0.51922) | -1 | -1 |
| G: -5312.08863 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.72023 HOMO: -6.18515 LUMO: -0.85988 factor:1 | 1 (-0.26591) | -1 | -1 |
| G: -5312.08863 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.50423 HOMO: -6.86815 LUMO: -1.90208 factor:1 | 1 (-0.04991) | -1 | -1 |
| G: -5312.08863 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.76668 HOMO: -6.37563 LUMO: -1.74697 factor:1 | 1 (-0.31236) | -1 | -1 |
| G: -5312.08863 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.78328 HOMO: -6.75659 LUMO: 0.36463 factor:1 | 1 (-0.32896) | -1 | -1 |
| G: -5312.08863 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.83596 HOMO: -6.91441 LUMO: -0.88981 factor:1 | 1 (-0.38164) | -1 | -1 |
| G: -5312.08863 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.87879 HOMO: -6.71305 LUMO: -0.29933 factor:1 | 1 (-0.42447) | -1 | -1 |
| G: -5312.08863 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.06726 HOMO: -6.91441 LUMO: -1.04492 factor:1 | 1 (-0.61294) | -1 | -1 |
| G: -5312.08863 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.90992 HOMO: -6.05453 LUMO: -0.83539 factor:1 | 1 (-0.45560) | -1 | -1 |
| G: -5312.08863 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.82649 HOMO: -7.35252 LUMO: -0.45715 factor:1 | 1 (-0.37217) | -1 | -1 |
| G: -5312.08863 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.70554 HOMO: -6.41644 LUMO: -0.97417 factor:1 | 1 (-0.25122) | -1 | -1 |
| G: -5312.08863 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.90200 HOMO: -6.78924 LUMO: 0.36735 factor:1 | 1 (-0.44768) | -1 | -1 |
| G: -5312.08863 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.74407 HOMO: -6.74298 LUMO: 0.51974 factor:1 | 1 (-0.28975) | -1 | -1 |
| G: -5312.08863 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.78516 HOMO: -6.48992 LUMO: 1.44765 factor:1 | 1 (-0.33084) | -1 | -1 |
| G: -5312.08863 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.54807 HOMO: -6.12528 LUMO: 1.57826 factor:1 | 1 (-0.09374) | -1 | -1 |
| G: -5312.08863 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.60782 HOMO: -6.62325 LUMO: 1.57826 factor:1 | 1 (-0.15350) | -1 | -1 |
| G: -5312.08863 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.43008 HOMO: -6.19875 LUMO: 1.29798 factor:1 | -1 (0.02425) | -1 | -1 |
| G: -5312.08863 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.74780 HOMO: -6.74570 LUMO: 1.52112 factor:1 | 1 (-0.29347) | -1 | -1 |
| G: -5312.08863 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.09861 HOMO: -6.84094 LUMO: 1.48574 factor:1 | 1 (-0.64428) | -1 | -1 |
| G: -5312.08863 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.96581 HOMO: -6.85183 LUMO: 0.33470 factor:1 | 1 (-0.51149) | -1 | -1 |
| G: -5312.08863 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.06669 HOMO: -6.51168 LUMO: 0.48164 factor:1 | 1 (-0.61237) | -1 | -1 |
| G: -5312.08863 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.95052 HOMO: -6.25046 LUMO: 0.75648 factor:1 | 1 (-0.49620) | -1 | -1 |
| G: -5312.08863 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.89381 HOMO: -6.65591 LUMO: 0.32109 factor:1 | 1 (-0.43949) | -1 | -1 |
| G: -5312.08863 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.75468 HOMO: -6.71033 LUMO: 0.40817 factor:1 | 1 (-0.30036) | -1 | -1 |
| G: -5312.08863 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.78323 HOMO: -6.75114 LUMO: 0.73471 factor:1 | 1 (-0.32890) | -1 | -1 |
| G: -5312.08863 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.71925 HOMO: -6.50624 LUMO: 0.59321 factor:1 | 1 (-0.26493) | -1 | -1 |
| G: -5312.08863 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.99975 HOMO: -6.39740 LUMO: 0.83267 factor:1 | 1 (-0.54543) | -1 | -1 |
| G: -5312.08863 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.68366 HOMO: -6.44094 LUMO: 0.65579 factor:1 | 1 (-0.22934) | -1 | -1 |
| G: -5312.08863 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.91482 HOMO: -6.52257 LUMO: 0.05714 factor:1 | 1 (-0.46050) | -1 | -1 |
| G: -5312.08863 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.63188 HOMO: -7.10217 LUMO: 0.49797 factor:1 | 1 (-0.17755) | -1 | -1 |
| G: -5312.08863 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.78793 HOMO: -6.83006 LUMO: 0.55783 factor:1 | 1 (-0.33361) | -1 | -1 |
| G: -5312.08863 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.48265 HOMO: -6.99333 LUMO: -0.79457 factor:1 | 1 (-0.02833) | -1 | -1 |
| G: -5312.08863 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.77427 HOMO: -6.64230 LUMO: 0.32382 factor:1 | 1 (-0.31995) | -1 | -1 |
| G: -5312.08863 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.60766 HOMO: -6.90897 LUMO: 0.30749 factor:1 | 1 (-0.15334) | -1 | -1 |
| G: -5312.08863 HOMO: -7.26544 LUMO: -1.10478 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.65694 HOMO: -7.09129 LUMO: 1.33336 factor:1 | 1 (-0.20262) | 1 | 1 |
| G: -5312.08863 HOMO: -7.26544 LUMO: -1.10478 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.39843 HOMO: -6.66951 LUMO: 1.34424 factor:1 | -1 (0.05589) | -1 | -1 |
| G: -5312.08863 HOMO: -7.26544 LUMO: -1.10478 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.97479 HOMO: -7.02870 LUMO: 1.48574 factor:1 | 1 (-0.52047) | -1 | -1 |
| G: -5312.08863 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.03743 HOMO: -7.26544 LUMO: 0.32926 factor:1 | 1 (-0.58311) | -1 | -1 |
| G: -5312.08863 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.13760 HOMO: -6.56067 LUMO: -0.45987 factor:1 | 1 (-0.68328) | -1 | -1 |
| G: -5312.08863 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.09050 HOMO: -6.54434 LUMO: -0.28300 factor:1 | 1 (-0.63617) | -1 | -1 |
| G: -5312.08863 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.11341 HOMO: -7.19469 LUMO: 0.54695 factor:1 | 1 (-0.65909) | -1 | -1 |
| G: -5312.08863 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.85264 HOMO: -6.47359 LUMO: -0.22041 factor:1 | 1 (-0.39832) | -1 | -1 |
| G: -5312.08863 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.86195 HOMO: -6.80013 LUMO: 2.08167 factor:1 | 1 (-0.40763) | -1 | -1 |
| G: -5312.08863 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.26843 HOMO: -6.23957 LUMO: 1.67894 factor:1 | 1 (-0.81411) | -1 | -1 |
| G: -5312.08863 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.09311 HOMO: -6.75114 LUMO: -0.62858 factor:1 | 1 (-0.63879) | -1 | -1 |
| G: -5312.08863 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.16642 HOMO: -6.79468 LUMO: -0.64491 factor:1 | 1 (-0.71209) | -1 | -1 |
| G: -5312.08863 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.03765 HOMO: -6.84911 LUMO: -0.69661 factor:1 | 1 (-0.58333) | -1 | -1 |
| G: -5312.08863 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.96701 HOMO: -7.54028 LUMO: 0.25851 factor:1 | 1 (-0.51269) | -1 | -1 |
| G: -5312.08863 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.95469 HOMO: -6.92802 LUMO: -0.71022 factor:1 | 1 (-0.50036) | -1 | -1 |
| G: -5312.08863 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.96048 HOMO: -6.72665 LUMO: -0.46804 factor:1 | 1 (-0.50616) | -1 | -1 |
| G: -5312.08863 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.07602 HOMO: -6.63686 LUMO: -0.23674 factor:1 | 1 (-0.62170) | -1 | -1 |
| G: -5312.08863 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.20103 HOMO: -7.21102 LUMO: 0.54423 factor:1 | 1 (-0.74671) | -1 | -1 |
| G: -5312.08863 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.24808 HOMO: -6.63414 LUMO: -0.25034 factor:1 | 1 (-0.79376) | -1 | -1 |
| G: -5312.08863 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.09031 HOMO: -6.70761 LUMO: -0.31837 factor:1 | 1 (-0.63598) | -1 | -1 |
| G: -5312.08863 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.04266 HOMO: -6.57155 LUMO: 1.76874 factor:1 | 1 (-0.58834) | -1 | -1 |
| G: -5312.08863 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.75539 HOMO: -6.84366 LUMO: 2.04358 factor:1 | 1 (-0.30107) | -1 | -1 |
| G: -5312.08863 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.75144 HOMO: -6.60420 LUMO: 1.80139 factor:1 | 1 (-0.29712) | -1 | -1 |
| G: -5312.08863 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.83623 HOMO: -7.03686 LUMO: 2.21229 factor:1 | 1 (-0.38191) | -1 | -1 |
| G: -5312.08863 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.10974 HOMO: -6.77564 LUMO: 1.97555 factor:1 | 1 (-0.65541) | -1 | -1 |
| G: -5312.08863 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.86965 HOMO: -6.40012 LUMO: 2.17691 factor:1 | 1 (-0.41533) | -1 | -1 |
| G: -5312.08863 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.16359 HOMO: -6.80013 LUMO: 2.25582 factor:1 | 1 (-0.70926) | -1 | -1 |
| G: -5312.08863 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.74208 HOMO: -6.74298 LUMO: 2.31569 factor:1 | 1 (-0.28776) | -1 | -1 |
| G: -5312.08863 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.93556 HOMO: -6.68856 LUMO: 1.85854 factor:1 | 1 (-0.48123) | -1 | -1 |
| G: -5312.08863 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.76067 HOMO: -6.17971 LUMO: 1.52928 factor:1 | 1 (-0.30635) | -1 | -1 |
| G: -5312.08863 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.54066 HOMO: -6.54162 LUMO: 1.91840 factor:1 | 1 (-0.08634) | -1 | -1 |
| G: -5312.08863 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.68371 HOMO: -6.80013 LUMO: -0.55511 factor:1 | 1 (-0.22939) | -1 | -1 |
| G: -5312.08863 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.86832 HOMO: -7.46953 LUMO: 0.28572 factor:1 | 1 (-0.41399) | -1 | -1 |
| G: -5312.08863 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.85022 HOMO: -6.61781 LUMO: -0.54967 factor:1 | 1 (-0.39590) | -1 | -1 |
| G: -5312.08863 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.12492 HOMO: -6.56339 LUMO: -0.47892 factor:1 | 1 (-0.67060) | -1 | -1 |
| G: -5312.08863 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.86192 HOMO: -6.65591 LUMO: -0.25307 factor:1 | 1 (-0.40760) | -1 | -1 |
| G: -5312.08863 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.96160 HOMO: -6.62869 LUMO: -0.23402 factor:1 | 1 (-0.50727) | -1 | -1 |
| G: -5312.08863 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.74148 HOMO: -6.58243 LUMO: -0.19048 factor:1 | 1 (-0.28716) | -1 | -1 |
| G: -5312.08863 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.05752 HOMO: -7.27632 LUMO: 0.52790 factor:1 | 1 (-0.60319) | -1 | -1 |
| G: -5312.08863 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.20187 HOMO: -7.21102 LUMO: 0.57688 factor:1 | 1 (-0.74755) | -1 | -1 |
| G: -5312.08863 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.82102 HOMO: -6.72393 LUMO: -0.53879 factor:1 | 1 (-0.36670) | -1 | -1 |
| G: -5312.08863 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.64412 HOMO: -7.42054 LUMO: -0.99322 factor:1 | 1 (-0.18980) | -1 | -1 |
| G: -5312.08863 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.94372 HOMO: -6.88992 LUMO: -0.71838 factor:1 | 1 (-0.48940) | -1 | -1 |
| G: -5312.08863 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.71166 HOMO: -6.88176 LUMO: -0.61226 factor:1 | 1 (-0.25734) | -1 | -1 |
| G: -5312.08863 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.63095 HOMO: -7.36340 LUMO: -1.04492 factor:1 | 1 (-0.17663) | -1 | -1 |
| G: -5312.08863 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.45688 HOMO: -6.65863 LUMO: -0.41906 factor:1 | 1 (-0.00256) | -1 | -1 |
| G: -5312.08863 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.96328 HOMO: -7.15115 LUMO: -0.66396 factor:1 | 1 (-0.50896) | -1 | -1 |
| G: -5312.08863 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.91428 HOMO: -7.10489 LUMO: -0.64491 factor:1 | 1 (-0.45995) | -1 | -1 |
| G: -5312.08863 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.16329 HOMO: -7.20285 LUMO: 0.47892 factor:1 | 1 (-0.70897) | -1 | -1 |
| G: -5312.08863 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.81452 HOMO: -6.55794 LUMO: -0.28844 factor:1 | 1 (-0.36020) | -1 | -1 |
| G: -5312.08863 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.68905 HOMO: -7.19197 LUMO: -0.69661 factor:1 | 1 (-0.23473) | -1 | -1 |
| G: -5312.08863 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.73563 HOMO: -6.56883 LUMO: -0.32926 factor:1 | 1 (-0.28131) | -1 | -1 |
| G: -5312.08863 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.96845 HOMO: -6.70761 LUMO: 1.95650 factor:1 | 1 (-0.51413) | -1 | -1 |
| G: -5312.08863 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.71142 HOMO: -6.60420 LUMO: 1.80684 factor:1 | 1 (-0.25709) | -1 | -1 |
| G: -5312.08863 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.72592 HOMO: -6.84094 LUMO: 1.64085 factor:1 | 1 (-0.27160) | -1 | -1 |
| G: -5312.08863 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.52129 HOMO: -6.69128 LUMO: 1.90208 factor:1 | 1 (-0.06697) | -1 | -1 |
| G: -5312.08863 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.59177 HOMO: -6.75387 LUMO: 1.70343 factor:1 | 1 (-0.13744) | -1 | -1 |
| G: -5312.08863 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.54140 HOMO: -7.07496 LUMO: 2.10072 factor:1 | 1 (-0.08708) | -1 | -1 |
| G: -5312.08863 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.32188 HOMO: -6.99877 LUMO: 2.24494 factor:1 | -1 (0.13244) | -1 | -1 |
| G: -5312.08863 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.75631 HOMO: -6.63414 LUMO: 2.17691 factor:1 | 1 (-0.30199) | -1 | -1 |
| G: -5312.08863 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.63870 HOMO: -6.44638 LUMO: 1.78235 factor:1 | 1 (-1.18438) | -1 | -1 |
| G: -5312.08863 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.80153 HOMO: -6.87632 LUMO: 1.84221 factor:1 | 1 (-1.34721) | -1 | -1 |
| G: -5312.08863 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.67432 HOMO: -6.85183 LUMO: 1.68711 factor:1 | 1 (-1.22000) | -1 | -1 |
| G: -5312.08863 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.73644 HOMO: -6.96339 LUMO: 2.26671 factor:1 | 1 (-1.28212) | -1 | -1 |
| G: -5312.08863 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.96877 HOMO: -6.63141 LUMO: 1.96738 factor:1 | 1 (-1.51445) | -1 | -1 |
| G: -5312.08863 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.95876 HOMO: -6.37019 LUMO: 2.23133 factor:1 | 1 (-1.50444) | -1 | -1 |
| G: -5312.08863 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.90872 HOMO: -7.11034 LUMO: 2.32385 factor:1 | 1 (-1.45439) | 1 | 1 |
| G: -5312.08863 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.92774 HOMO: -6.91986 LUMO: 1.65445 factor:1 | 1 (-1.47341) | -1 | -1 |
| G: -5312.08863 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.65769 HOMO: -7.12938 LUMO: 2.28304 factor:1 | 1 (-1.20337) | 1 | 1 |
| G: -5312.08863 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.63043 HOMO: -6.54978 LUMO: 1.92112 factor:1 | 1 (-1.17610) | -1 | -1 |
| G: -5312.08863 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.45026 HOMO: -6.83006 LUMO: 2.48712 factor:1 | 1 (-0.99594) | -1 | -1 |
| G: -5312.08863 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.56498 HOMO: -6.97972 LUMO: 1.96738 factor:1 | 1 (-1.11066) | -1 | -1 |
| G: -5312.08863 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.49097 HOMO: -6.69944 LUMO: 2.06262 factor:1 | 1 (-1.03664) | -1 | -1 |
| G: -5312.08863 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.48065 HOMO: -6.76747 LUMO: 2.10888 factor:1 | 1 (-1.02633) | -1 | -1 |
| G: -5312.08863 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.65290 HOMO: -6.91169 LUMO: 2.06534 factor:1 | 1 (-1.19858) | -1 | -1 |
| G: -5312.08863 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.98152 HOMO: -7.03414 LUMO: 1.93473 factor:1 | 1 (-0.52719) | -1 | -1 |
| G: -5312.08863 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.05708 HOMO: -7.03142 LUMO: 2.52250 factor:1 | 1 (-0.60276) | -1 | -1 |
| G: -5312.08863 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.11439 HOMO: -6.34025 LUMO: 2.61229 factor:1 | 1 (-0.66007) | -1 | -1 |
| G: -5312.08863 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.17559 HOMO: -6.98788 LUMO: 2.28304 factor:1 | 1 (-0.72126) | -1 | -1 |
| G: -5312.08863 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.18280 HOMO: -6.97700 LUMO: 2.53882 factor:1 | 1 (-0.72848) | -1 | -1 |
| G: -5312.08863 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.11270 HOMO: -6.58788 LUMO: 1.94289 factor:1 | 1 (-0.65838) | -1 | -1 |
| G: -5312.08863 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.90410 HOMO: -6.78652 LUMO: 2.13609 factor:1 | 1 (-0.44978) | -1 | -1 |
| G: -5312.08863 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.87038 HOMO: -6.55250 LUMO: 1.82861 factor:1 | 1 (-0.41606) | -1 | -1 |
| G: -5312.08863 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.75283 HOMO: -6.45998 LUMO: 1.75786 factor:1 | 1 (-0.29851) | -1 | -1 |
| G: -5312.08863 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.90707 HOMO: -6.78924 LUMO: 2.33746 factor:1 | 1 (-0.45274) | -1 | -1 |
| G: -5312.08863 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.67103 HOMO: -6.85727 LUMO: 1.76058 factor:1 | 1 (-0.21671) | -1 | -1 |
| G: -5312.08863 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.89659 HOMO: -6.70489 LUMO: 1.84493 factor:1 | 1 (-0.44227) | -1 | -1 |
| G: -5312.08863 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.69893 HOMO: -6.71305 LUMO: 1.53472 factor:1 | 1 (-0.24460) | -1 | -1 |
| G: -5312.08863 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.93077 HOMO: -6.76747 LUMO: 1.48846 factor:1 | 1 (-0.47644) | -1 | -1 |
| G: -5312.08863 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.89904 HOMO: -6.69128 LUMO: 1.95922 factor:1 | 1 (-0.44472) | -1 | -1 |
| G: -5312.08863 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.77642 HOMO: -6.67495 LUMO: 2.05446 factor:1 | 1 (-0.32210) | -1 | -1 |
| G: -5312.08863 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.86100 HOMO: -6.63686 LUMO: 2.25310 factor:1 | 1 (-0.40667) | -1 | -1 |
| G: -5312.08863 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.59930 HOMO: -6.63958 LUMO: 2.14154 factor:1 | 1 (-0.14498) | -1 | -1 |
| G: -5312.08863 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.92663 HOMO: -6.62597 LUMO: 2.01908 factor:1 | 1 (-0.47231) | -1 | -1 |
| G: -5312.08863 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.68611 HOMO: -7.07768 LUMO: 2.14154 factor:1 | 1 (-0.23179) | -1 | -1 |
| G: -5312.08863 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.55683 HOMO: -6.19603 LUMO: 2.01092 factor:1 | 1 (-0.10251) | -1 | -1 |
| G: -5312.08863 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.51397 HOMO: -6.65046 LUMO: 2.15786 factor:1 | 1 (-0.05965) | -1 | -1 |
| G: -5312.08863 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.76355 HOMO: -6.92258 LUMO: 2.31841 factor:1 | 1 (-0.30923) | -1 | -1 |
| G: -5312.08863 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.57638 HOMO: -6.90081 LUMO: 2.19324 factor:1 | 1 (-1.12206) | -1 | -1 |
| G: -5312.08863 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.40958 HOMO: -6.85455 LUMO: 1.95650 factor:1 | 1 (-0.95526) | -1 | -1 |
| G: -5312.08863 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.54188 HOMO: -6.57699 LUMO: 1.76058 factor:1 | 1 (-1.08756) | -1 | -1 |
| G: -5312.08863 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.58384 HOMO: -6.90625 LUMO: 1.97555 factor:1 | 1 (-1.12952) | -1 | -1 |
| G: -5312.08863 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.70945 HOMO: -6.97428 LUMO: 1.92929 factor:1 | 1 (-1.25513) | -1 | -1 |
| G: -5312.08863 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.77786 HOMO: -6.61781 LUMO: -0.41906 factor:1 | 1 (-1.32353) | -1 | -1 |
| G: -5312.08863 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.55861 HOMO: -6.62869 LUMO: -0.81906 factor:1 | 1 (-1.10429) | -1 | -1 |
| G: -5312.08863 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.61418 HOMO: -7.01237 LUMO: 2.00548 factor:1 | 1 (-1.15986) | -1 | -1 |
| G: -5312.08863 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.50438 HOMO: -6.85727 LUMO: 2.17691 factor:1 | 1 (-1.05006) | -1 | -1 |
| G: -5312.08863 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.91176 HOMO: -6.71849 LUMO: 1.58914 factor:1 | 1 (-1.45744) | -1 | -1 |
| G: -5312.08863 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.48765 HOMO: -7.52395 LUMO: 0.27211 factor:1 | 1 (-1.03333) | -1 | -1 |
| G: -5312.08863 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.36862 HOMO: -6.96611 LUMO: -0.72654 factor:1 | 1 (-0.91430) | -1 | -1 |
| G: -5312.08863 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.25153 HOMO: -6.89537 LUMO: -0.68028 factor:1 | 1 (-0.79721) | -1 | -1 |
| G: -5312.08863 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.34509 HOMO: -6.84911 LUMO: -0.58504 factor:1 | 1 (-0.89076) | -1 | -1 |
| G: -5312.08863 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.64632 HOMO: -6.79196 LUMO: -0.55783 factor:1 | 1 (-1.19199) | -1 | -1 |
| G: -5312.08863 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.79182 HOMO: -6.67767 LUMO: 1.79323 factor:1 | 1 (-1.33749) | -1 | -1 |
| G: -5312.08863 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.57162 HOMO: -6.54434 LUMO: 1.91024 factor:1 | 1 (-1.11730) | -1 | -1 |
| G: -5312.08863 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.62871 HOMO: -6.62869 LUMO: 1.69799 factor:1 | 1 (-1.17439) | -1 | -1 |
| G: -5312.08863 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.87715 HOMO: -6.72393 LUMO: 2.12249 factor:1 | 1 (-1.42283) | -1 | -1 |
| G: -5312.08863 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.87813 HOMO: -6.66407 LUMO: 2.05990 factor:1 | 1 (-1.42381) | -1 | -1 |
| G: -5312.08863 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.57652 HOMO: -7.00149 LUMO: 1.82044 factor:1 | 1 (-1.12220) | -1 | -1 |
| G: -5312.08863 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.59940 HOMO: -7.12122 LUMO: 2.16058 factor:1 | 1 (-1.14508) | 1 | 1 |
| G: -5312.08863 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.48025 HOMO: -6.63141 LUMO: 2.21229 factor:1 | 1 (-1.02592) | -1 | -1 |
| G: -5312.08863 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.39891 HOMO: -6.37835 LUMO: 2.32113 factor:1 | 1 (-0.94459) | -1 | -1 |
| G: -5312.08863 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.41015 HOMO: -6.99605 LUMO: 2.00548 factor:1 | 1 (-0.95583) | -1 | -1 |
| G: -5312.08863 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.72392 HOMO: -6.85999 LUMO: 2.39460 factor:1 | 1 (-1.26960) | -1 | -1 |
| G: -5312.08863 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.55203 HOMO: -6.85727 LUMO: 2.48712 factor:1 | 1 (-1.09771) | -1 | -1 |
| G: -5312.08863 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.55497 HOMO: -7.04231 LUMO: 2.40277 factor:1 | 1 (-1.10065) | -1 | -1 |
| G: -5312.08863 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11578.15727 HOMO: -6.60692 LUMO: 2.26671 factor:1 | 1 (-1.70294) | -1 | -1 |
| G: -5312.08863 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11578.38769 HOMO: -6.67495 LUMO: 2.14698 factor:1 | 1 (-1.93337) | -1 | -1 |
| G: -5312.08863 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11578.98297 HOMO: -6.73210 LUMO: 2.06807 factor:1 | 1 (-2.52865) | -1 | -1 |
| G: -5312.08863 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.97255 HOMO: -7.20013 LUMO: 2.02181 factor:1 | 1 (-1.51823) | 1 | 1 |
| G: -5312.08863 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.96265 HOMO: -7.18653 LUMO: 2.29936 factor:1 | 1 (-1.50833) | 1 | 1 |
| G: -5312.08863 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11578.18861 HOMO: -6.92802 LUMO: 2.36195 factor:1 | 1 (-1.73429) | -1 | -1 |
| G: -5312.08863 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.99873 HOMO: -6.89537 LUMO: 1.78779 factor:1 | 1 (-1.54441) | -1 | -1 |
| G: -5312.08863 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.96820 HOMO: -6.96067 LUMO: 2.31297 factor:1 | 1 (-1.51388) | -1 | -1 |
| G: -5312.08863 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11578.19425 HOMO: -6.91441 LUMO: 2.50345 factor:1 | 1 (-1.73992) | -1 | -1 |
| G: -5312.08863 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.83141 HOMO: -7.17292 LUMO: 2.12521 factor:1 | 1 (-1.37709) | 1 | 1 |
| G: -5312.08863 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11578.98033 HOMO: -6.93618 LUMO: 2.35106 factor:1 | 1 (-2.52601) | -1 | -1 |
| G: -5312.08863 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11578.98218 HOMO: -6.75931 LUMO: 1.61908 factor:1 | 1 (-2.52786) | -1 | -1 |
| G: -5312.08863 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.79497 HOMO: -6.35930 LUMO: 1.23540 factor:1 | 1 (-1.34065) | -1 | -1 |
| G: -5312.08863 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11578.00496 HOMO: -6.17971 LUMO: 1.84493 factor:1 | 1 (-1.55064) | -1 | -1 |
| G: -5312.08863 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.93108 HOMO: -6.72665 LUMO: 2.61229 factor:1 | 1 (-1.47676) | -1 | -1 |
| G: -5312.08863 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.82882 HOMO: -6.62869 LUMO: 2.28304 factor:1 | 1 (-1.37450) | -1 | -1 |
| G: -5312.08863 HOMO: -8.88180 LUMO: 1.02315 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.58974 HOMO: -6.58243 LUMO: 0.28028 factor:1 | 1 (-1.13542) | -1 | -1 |
| G: -5312.08863 HOMO: -8.88180 LUMO: 1.02315 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11578.11101 HOMO: -6.79468 LUMO: 0.14966 factor:1 | 1 (-1.65668) | -1 | -1 |
| G: -5312.08863 HOMO: -8.88180 LUMO: 1.02315 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11578.38206 HOMO: -6.63141 LUMO: 0.31021 factor:1 | 1 (-1.92774) | -1 | -1 |
| G: -5312.08863 HOMO: -8.88180 LUMO: 1.02315 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11578.12611 HOMO: -6.81101 LUMO: 0.13878 factor:1 | 1 (-1.67179) | -1 | -1 |
| G: -5312.08863 HOMO: -8.88180 LUMO: 1.02315 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11578.10246 HOMO: -6.72665 LUMO: 0.65579 factor:1 | 1 (-1.64814) | -1 | -1 |
| G: -5312.08863 HOMO: -8.88180 LUMO: 1.02315 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.89930 HOMO: -6.53073 LUMO: 0.91430 factor:1 | 1 (-1.44498) | -1 | -1 |
| G: -5312.08863 HOMO: -8.88180 LUMO: 1.02315 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.80412 HOMO: -7.19197 LUMO: 1.62996 factor:1 | 1 (-0.34980) | 1 | 1 |
| G: -5312.08863 HOMO: -8.88180 LUMO: 1.02315 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.83515 HOMO: -6.69400 LUMO: 0.84627 factor:1 | 1 (-0.38082) | -1 | -1 |
| G: -5312.08863 HOMO: -8.88180 LUMO: 1.02315 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.02075 HOMO: -6.76475 LUMO: 0.51974 factor:1 | 1 (-0.56643) | -1 | -1 |
| G: -5312.08863 HOMO: -8.88180 LUMO: 1.02315 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.78886 HOMO: -6.67767 LUMO: 0.52246 factor:1 | 1 (-0.33454) | -1 | -1 |
| G: -5312.08863 HOMO: -8.88180 LUMO: 1.02315 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.73950 HOMO: -6.73210 LUMO: 0.94424 factor:1 | 1 (-0.28518) | -1 | -1 |
| G: -5312.08863 HOMO: -8.88180 LUMO: 1.02315 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.80244 HOMO: -6.97972 LUMO: 0.60409 factor:1 | 1 (-0.34812) | -1 | -1 |
| G: -5312.08863 HOMO: -8.88180 LUMO: 1.02315 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.59253 HOMO: -7.38517 LUMO: 0.73743 factor:1 | 1 (-0.13821) | -1 | -1 |
| G: -5312.08863 HOMO: -8.88180 LUMO: 1.02315 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.69710 HOMO: -6.48992 LUMO: 1.08301 factor:1 | 1 (-0.24278) | -1 | -1 |
| G: -5312.08863 HOMO: -8.88180 LUMO: 1.02315 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.88628 HOMO: -7.18381 LUMO: 1.61908 factor:1 | 1 (-0.43195) | 1 | 1 |
| G: -5312.08863 HOMO: -8.88180 LUMO: 1.02315 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.77851 HOMO: -6.74842 LUMO: 0.57960 factor:1 | 1 (-1.32419) | -1 | -1 |
| G: -5312.08863 HOMO: -8.88180 LUMO: 1.02315 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11578.60606 HOMO: -6.67495 LUMO: 0.77280 factor:1 | 1 (-2.15174) | -1 | -1 |
| G: -5312.08863 HOMO: -8.88180 LUMO: 1.02315 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.94219 HOMO: -6.74570 LUMO: 0.77280 factor:1 | 1 (-1.48786) | -1 | -1 |
| G: -5312.08863 HOMO: -8.88180 LUMO: 1.02315 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.83549 HOMO: -6.73754 LUMO: 0.86804 factor:1 | 1 (-1.38117) | -1 | -1 |
| G: -5312.08863 HOMO: -8.88180 LUMO: 1.02315 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.77712 HOMO: -6.66135 LUMO: 0.94424 factor:1 | 1 (-1.32280) | -1 | -1 |
| G: -5312.08863 HOMO: -8.88180 LUMO: 1.02315 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.57110 HOMO: -6.44638 LUMO: 1.00138 factor:1 | 1 (-1.11678) | -1 | -1 |
| G: -5312.08863 HOMO: -8.88180 LUMO: 1.02315 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.80442 HOMO: -6.65591 LUMO: 1.02043 factor:1 | 1 (-1.35009) | -1 | -1 |
| G: -5312.08863 HOMO: -8.88180 LUMO: 1.02315 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.61530 HOMO: -7.17564 LUMO: 0.50069 factor:1 | 1 (-1.16097) | -1 | -1 |
| G: -5312.08863 HOMO: -8.88180 LUMO: 1.02315 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.80771 HOMO: -6.59332 LUMO: 0.79457 factor:1 | 1 (-1.35339) | -1 | -1 |
| G: -5312.08863 HOMO: -8.88180 LUMO: 1.02315 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.65108 HOMO: -6.76747 LUMO: 1.73881 factor:1 | 1 (-1.19676) | -1 | -1 |
| G: -5312.08863 HOMO: -8.88180 LUMO: 1.02315 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.80096 HOMO: -7.00421 LUMO: 1.07485 factor:1 | 1 (-1.34664) | -1 | -1 |
| G: -5312.08863 HOMO: -8.88180 LUMO: 1.02315 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.76194 HOMO: -6.94979 LUMO: 1.67894 factor:1 | 1 (-1.30762) | -1 | -1 |
| G: -5312.08863 HOMO: -8.88180 LUMO: 1.02315 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.88070 HOMO: -6.66135 LUMO: 0.47076 factor:1 | 1 (-0.42638) | -1 | -1 |
| G: -5312.08863 HOMO: -8.88180 LUMO: 1.02315 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.90424 HOMO: -6.74298 LUMO: 1.85037 factor:1 | 1 (-0.44991) | -1 | -1 |
| G: -5312.08863 HOMO: -8.88180 LUMO: 1.02315 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.00598 HOMO: -6.65318 LUMO: 0.95240 factor:1 | 1 (-0.55166) | -1 | -1 |
| G: -5312.08863 HOMO: -8.88180 LUMO: 1.02315 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.12816 HOMO: -6.63958 LUMO: 0.78097 factor:1 | 1 (-0.67384) | -1 | -1 |
| G: -5312.08863 HOMO: -8.88180 LUMO: 1.02315 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.02026 HOMO: -6.11712 LUMO: 0.40001 factor:1 | 1 (-0.56594) | -1 | -1 |
| G: -5312.08863 HOMO: -8.88180 LUMO: 1.02315 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.92772 HOMO: -7.08312 LUMO: 0.92519 factor:1 | 1 (-0.47340) | -1 | -1 |
| G: -5312.08863 HOMO: -8.88180 LUMO: 1.02315 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.90870 HOMO: -6.96067 LUMO: 0.54695 factor:1 | 1 (-0.45438) | -1 | -1 |
| G: -5312.08863 HOMO: -8.88180 LUMO: 1.02315 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.04040 HOMO: -6.74026 LUMO: 0.60137 factor:1 | 1 (-0.58608) | -1 | -1 |
| G: -5312.08863 HOMO: -8.88180 LUMO: 1.02315 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.96747 HOMO: -6.74298 LUMO: 0.59593 factor:1 | 1 (-0.51315) | -1 | -1 |
| G: -5312.08863 HOMO: -8.88180 LUMO: 1.02315 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.68956 HOMO: -6.93074 LUMO: 0.60681 factor:1 | 1 (-0.23524) | -1 | -1 |
| G: -5312.08863 HOMO: -8.88180 LUMO: 1.02315 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.93128 HOMO: -6.41644 LUMO: 0.35919 factor:1 | 1 (-0.47696) | -1 | -1 |
| G: -5312.08863 HOMO: -8.88180 LUMO: 1.02315 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.76001 HOMO: -6.41917 LUMO: 1.73064 factor:1 | 1 (-0.30569) | -1 | -1 |
| G: -5312.08863 HOMO: -8.88180 LUMO: 1.02315 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.96421 HOMO: -4.64226 LUMO: -0.87893 factor:1 | 1 (-0.50989) | -1 | -1 |
| G: -5312.08863 HOMO: -8.88180 LUMO: 1.02315 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.01020 HOMO: -6.59604 LUMO: 0.90342 factor:1 | 1 (-0.55587) | -1 | -1 |
| G: -5312.08863 HOMO: -8.88180 LUMO: 1.02315 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.77836 HOMO: -6.79468 LUMO: 0.50069 factor:1 | 1 (-0.32403) | -1 | -1 |
| G: -5312.08863 HOMO: -8.88180 LUMO: 1.02315 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.00339 HOMO: -7.04503 LUMO: 0.52518 factor:1 | 1 (-0.54907) | -1 | -1 |
| G: -5312.08863 HOMO: -8.88180 LUMO: 1.02315 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.81721 HOMO: -6.69400 LUMO: 0.54423 factor:1 | 1 (-0.36289) | -1 | -1 |
| G: -5312.08863 HOMO: -8.88180 LUMO: 1.02315 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.98712 HOMO: -6.51713 LUMO: 0.95240 factor:1 | 1 (-0.53280) | -1 | -1 |
| G: -5312.08863 HOMO: -8.88180 LUMO: 1.02315 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.77871 HOMO: -6.88176 LUMO: 1.79323 factor:1 | 1 (-0.32439) | -1 | -1 |
| G: -5312.08863 HOMO: -8.88180 LUMO: 1.02315 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.09684 HOMO: -6.71849 LUMO: 0.28844 factor:1 | 1 (-0.64252) | -1 | -1 |
| G: -5312.08863 HOMO: -8.88180 LUMO: 1.02315 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.80837 HOMO: -6.94979 LUMO: 0.51974 factor:1 | 1 (-0.35405) | -1 | -1 |
| G: -5312.08863 HOMO: -8.88180 LUMO: 1.02315 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.56178 HOMO: -6.76203 LUMO: 0.94151 factor:1 | 1 (-0.10746) | -1 | -1 |
| G: -5312.08863 HOMO: -8.88180 LUMO: 1.02315 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.81928 HOMO: -6.91169 LUMO: 0.89525 factor:1 | 1 (-0.36496) | -1 | -1 |
| G: -5312.08863 HOMO: -8.88180 LUMO: 1.02315 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.04212 HOMO: -6.83006 LUMO: 0.89253 factor:1 | 1 (-0.58779) | -1 | -1 |
| G: -5312.08863 HOMO: -8.88180 LUMO: 1.02315 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.84208 HOMO: -7.08857 LUMO: 0.60409 factor:1 | 1 (-0.38776) | -1 | -1 |
| G: -5312.08863 HOMO: -8.88180 LUMO: 1.02315 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.93322 HOMO: -6.91713 LUMO: 1.76330 factor:1 | 1 (-0.47889) | -1 | -1 |
| G: -5312.08863 HOMO: -8.88180 LUMO: 1.02315 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.72227 HOMO: -6.47359 LUMO: 1.56193 factor:1 | 1 (-0.26795) | -1 | -1 |
| G: -5312.08863 HOMO: -6.91169 LUMO: -0.53879 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.04337 HOMO: -7.00149 LUMO: 1.47214 factor:1 | 1 (-0.58904) | -1 | -1 |
| G: -5312.08863 HOMO: -6.91169 LUMO: -0.53879 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.83278 HOMO: -7.03686 LUMO: 1.97283 factor:1 | 1 (-0.37846) | -1 | -1 |
| G: -5312.08863 HOMO: -6.91169 LUMO: -0.53879 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.79207 HOMO: -7.00965 LUMO: 1.64629 factor:1 | 1 (-0.33775) | -1 | -1 |
| G: -5312.08863 HOMO: -6.91169 LUMO: -0.53879 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.51941 HOMO: -7.06952 LUMO: 1.67622 factor:1 | 1 (-0.06509) | 1 | -1 |
| G: -5312.08863 HOMO: -6.91169 LUMO: -0.53879 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.88617 HOMO: -6.80557 LUMO: 1.70615 factor:1 | 1 (-0.43184) | -1 | -1 |
| G: -5312.08863 HOMO: -6.91169 LUMO: -0.53879 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.62926 HOMO: -6.80829 LUMO: 1.71704 factor:1 | 1 (-0.17494) | -1 | -1 |
| G: -5312.08863 HOMO: -6.91169 LUMO: -0.53879 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.44537 HOMO: -7.26544 LUMO: 1.89935 factor:1 | -1 (0.00895) | 1 | -1 |
| G: -5312.08863 HOMO: -7.29809 LUMO: 2.83543 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.64423 HOMO: -7.00149 LUMO: 1.47214 factor:1 | 1 (-0.18991) | -1 | -1 |
| G: -5312.08863 HOMO: -7.29809 LUMO: 2.83543 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.80597 HOMO: -7.03686 LUMO: 1.97283 factor:1 | 1 (-0.35165) | -1 | -1 |
| G: -5312.08863 HOMO: -7.29809 LUMO: 2.83543 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.78347 HOMO: -7.00965 LUMO: 1.64629 factor:1 | 1 (-0.32915) | -1 | -1 |
| G: -5312.08863 HOMO: -7.29809 LUMO: 2.83543 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.83830 HOMO: -7.06952 LUMO: 1.67622 factor:1 | 1 (-0.38398) | -1 | -1 |
| G: -5312.08863 HOMO: -7.29809 LUMO: 2.83543 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.88540 HOMO: -6.80557 LUMO: 1.70615 factor:1 | 1 (-0.43108) | -1 | -1 |
| G: -5312.08863 HOMO: -7.29809 LUMO: 2.83543 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.79493 HOMO: -6.80829 LUMO: 1.71704 factor:1 | 1 (-0.34060) | -1 | -1 |
| G: -5312.08863 HOMO: -7.29809 LUMO: 2.83543 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.75939 HOMO: -7.26544 LUMO: 1.89935 factor:1 | 1 (-0.30507) | -1 | -1 |
| G: -5312.08863 HOMO: -7.85865 LUMO: 2.83543 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.79498 HOMO: -7.00149 LUMO: 1.75241 factor:1 | 1 (-0.34066) | -1 | -1 |
| G: -5312.08863 HOMO: -7.85865 LUMO: 2.83543 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.94500 HOMO: -6.91169 LUMO: 2.07079 factor:1 | 1 (-0.49068) | -1 | -1 |
| G: -5312.08863 HOMO: -7.85865 LUMO: 2.83543 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.10780 HOMO: -7.11034 LUMO: 1.76330 factor:1 | 1 (-0.65348) | -1 | -1 |
| G: -5312.08863 HOMO: -7.85865 LUMO: 2.83543 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.96911 HOMO: -6.87360 LUMO: 2.02725 factor:1 | 1 (-0.51479) | -1 | -1 |
| G: -5312.08863 HOMO: -7.85865 LUMO: 2.83543 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.01485 HOMO: -7.08584 LUMO: 1.82044 factor:1 | 1 (-0.56053) | -1 | -1 |
| G: -5312.08863 HOMO: -7.85865 LUMO: 2.83543 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.94728 HOMO: -6.90625 LUMO: 1.68166 factor:1 | 1 (-0.49296) | -1 | -1 |
| G: -5312.08863 HOMO: -7.85865 LUMO: 2.83543 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.91156 HOMO: -6.71577 LUMO: 1.93201 factor:1 | 1 (-0.45723) | -1 | -1 |
| G: -5312.08863 HOMO: -7.85865 LUMO: 2.83543 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.79046 HOMO: -6.99605 LUMO: 2.08439 factor:1 | 1 (-0.33614) | -1 | -1 |
| G: -5312.08863 HOMO: -7.85865 LUMO: 2.83543 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.98707 HOMO: -7.02326 LUMO: 1.97010 factor:1 | 1 (-0.53274) | -1 | -1 |
| G: -5312.08863 HOMO: -7.85865 LUMO: 2.83543 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.87191 HOMO: -6.99877 LUMO: 2.15514 factor:1 | 1 (-0.41759) | -1 | -1 |
| G: -5312.08863 HOMO: -7.85865 LUMO: 2.83543 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.15814 HOMO: -6.75387 LUMO: 1.95106 factor:1 | 1 (-0.70382) | -1 | -1 |
| G: -5312.08863 HOMO: -7.85865 LUMO: 2.83543 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.97226 HOMO: -7.10761 LUMO: 2.06262 factor:1 | 1 (-0.51794) | -1 | -1 |
| G: -5312.08863 HOMO: -7.85865 LUMO: 2.83543 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.93123 HOMO: -7.03142 LUMO: 1.91568 factor:1 | 1 (-0.47691) | -1 | -1 |
| G: -5312.08863 HOMO: -7.85865 LUMO: 2.83543 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.89789 HOMO: -6.98788 LUMO: 1.98371 factor:1 | 1 (-0.44357) | -1 | -1 |
| G: -5312.08863 HOMO: -7.85865 LUMO: 2.83543 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.04990 HOMO: -6.94707 LUMO: 1.68438 factor:1 | 1 (-0.59558) | -1 | -1 |
| G: -5312.08863 HOMO: -7.85865 LUMO: 2.83543 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.78608 HOMO: -6.88176 LUMO: 2.20684 factor:1 | 1 (-0.33176) | -1 | -1 |
| G: -5312.08863 HOMO: -7.85865 LUMO: 2.83543 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.96845 HOMO: -6.73210 LUMO: 2.18780 factor:1 | 1 (-0.51413) | -1 | -1 |
| G: -5312.08863 HOMO: -7.85865 LUMO: 2.83543 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.77359 HOMO: -6.83822 LUMO: 2.06807 factor:1 | 1 (-0.31927) | -1 | -1 |
| G: -5312.08863 HOMO: -7.85865 LUMO: 2.83543 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.96737 HOMO: -6.78924 LUMO: 2.42181 factor:1 | 1 (-0.51304) | -1 | -1 |
| G: -5312.08863 HOMO: -7.85865 LUMO: 2.83543 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.77528 HOMO: -6.94707 LUMO: 1.71704 factor:1 | 1 (-0.32096) | -1 | -1 |
| G: -5312.08863 HOMO: -7.85865 LUMO: 2.83543 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.98138 HOMO: -6.85183 LUMO: 1.78779 factor:1 | 1 (-0.52706) | -1 | -1 |
| G: -5312.08863 HOMO: -7.85865 LUMO: 2.83543 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.81403 HOMO: -6.98788 LUMO: 1.69799 factor:1 | 1 (-0.35971) | -1 | -1 |
| G: -5312.08863 HOMO: -7.85865 LUMO: 2.83543 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.43704 HOMO: -6.79468 LUMO: 2.04358 factor:1 | -1 (0.01728) | -1 | -1 |
| G: -5312.08863 HOMO: -7.85865 LUMO: 2.83543 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.65620 HOMO: -6.90081 LUMO: 1.97283 factor:1 | 1 (-0.20188) | -1 | -1 |
| G: -5312.08863 HOMO: -7.85865 LUMO: 2.83543 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.51533 HOMO: -6.79468 LUMO: 2.00820 factor:1 | 1 (-0.06101) | -1 | -1 |
| G: -5312.08863 HOMO: -7.85865 LUMO: 2.83543 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.85691 HOMO: -7.06408 LUMO: 2.29936 factor:1 | 1 (-0.40259) | -1 | -1 |
| G: -5312.08863 HOMO: -7.85865 LUMO: 2.83543 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.58203 HOMO: -6.78924 LUMO: 2.13337 factor:1 | 1 (-0.12770) | -1 | -1 |
| G: -5312.08863 HOMO: -7.85865 LUMO: 2.83543 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.54646 HOMO: -6.79468 LUMO: 2.35106 factor:1 | 1 (-0.09214) | -1 | -1 |
| G: -5312.08863 HOMO: -7.85865 LUMO: 2.83543 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.38580 HOMO: -6.82734 LUMO: 2.16603 factor:1 | -1 (0.06852) | -1 | -1 |
| G: -5312.08863 HOMO: -7.85865 LUMO: 2.83543 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.73158 HOMO: -6.79740 LUMO: 2.36739 factor:1 | 1 (-0.27726) | -1 | -1 |
| G: -5312.08863 HOMO: -7.85865 LUMO: 2.83543 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.91675 HOMO: -7.14027 LUMO: 2.10888 factor:1 | 1 (-0.46243) | -1 | -1 |
| G: -5312.08863 HOMO: -6.61509 LUMO: -0.23674 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.91068 HOMO: -6.96067 LUMO: 1.59731 factor:1 | 1 (-0.45636) | -1 | -1 |
| G: -5312.08863 HOMO: -6.61509 LUMO: -0.23674 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.89278 HOMO: -6.91169 LUMO: 1.37145 factor:1 | 1 (-0.43846) | -1 | -1 |
| G: -5312.08863 HOMO: -6.61509 LUMO: -0.23674 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.01104 HOMO: -6.94707 LUMO: 1.73064 factor:1 | 1 (-0.55672) | -1 | -1 |
| G: -5312.08863 HOMO: -6.61509 LUMO: -0.23674 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.03980 HOMO: -7.02326 LUMO: 1.41227 factor:1 | 1 (-0.58548) | -1 | -1 |
| G: -5312.08863 HOMO: -6.61509 LUMO: -0.23674 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.92524 HOMO: -6.72121 LUMO: 1.43132 factor:1 | 1 (-0.47092) | -1 | -1 |
| G: -5312.08863 HOMO: -6.61509 LUMO: -0.23674 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.88745 HOMO: -6.51168 LUMO: 1.72520 factor:1 | 1 (-0.43312) | -1 | -1 |
| G: -5312.08863 HOMO: -6.61509 LUMO: -0.23674 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.84663 HOMO: -6.98516 LUMO: 1.92929 factor:1 | 1 (-0.39231) | -1 | -1 |
| G: -5312.08863 HOMO: -6.61509 LUMO: -0.23674 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.82842 HOMO: -6.92802 LUMO: 2.07895 factor:1 | 1 (-0.37410) | -1 | -1 |
| G: -5312.08863 HOMO: -6.61509 LUMO: -0.23674 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.72116 HOMO: -7.02326 LUMO: 1.86398 factor:1 | 1 (-0.26683) | -1 | -1 |
| G: -5312.08863 HOMO: -6.61509 LUMO: -0.23674 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.69435 HOMO: -6.82462 LUMO: 1.86670 factor:1 | 1 (-0.24003) | -1 | -1 |
| G: -5312.08863 HOMO: -6.61509 LUMO: -0.23674 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.71814 HOMO: -6.83278 LUMO: 1.71160 factor:1 | 1 (-0.26381) | -1 | -1 |
| G: -5312.08863 HOMO: -6.61509 LUMO: -0.23674 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.92380 HOMO: -6.62869 LUMO: 1.69527 factor:1 | 1 (-0.46948) | -1 | -1 |
| G: -5312.08863 HOMO: -6.61509 LUMO: -0.23674 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.67005 HOMO: -6.84094 LUMO: 1.27349 factor:1 | 1 (-1.21572) | -1 | -1 |
| G: -5312.08863 HOMO: -6.61509 LUMO: -0.23674 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.79258 HOMO: -7.07768 LUMO: 1.27621 factor:1 | 1 (-1.33826) | 1 | -1 |
| G: -5312.08863 HOMO: -6.61509 LUMO: -0.23674 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.86420 HOMO: -7.06135 LUMO: 1.55105 factor:1 | 1 (-1.40988) | 1 | -1 |
| G: -5312.08863 HOMO: -6.61509 LUMO: -0.23674 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.47829 HOMO: -6.94162 LUMO: 1.64629 factor:1 | 1 (-1.02396) | -1 | -1 |
| G: -5312.08863 HOMO: -6.61509 LUMO: -0.23674 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.43505 HOMO: -7.07224 LUMO: 1.65445 factor:1 | 1 (-0.98073) | 1 | -1 |
| G: -5312.08863 HOMO: -6.61509 LUMO: -0.23674 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.44961 HOMO: -6.68584 LUMO: 1.91296 factor:1 | 1 (-0.99528) | -1 | -1 |
| G: -5312.08863 HOMO: -6.61509 LUMO: -0.23674 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.43265 HOMO: -7.09129 LUMO: 1.73609 factor:1 | 1 (-0.97833) | 1 | -1 |
| G: -5312.08863 HOMO: -6.61509 LUMO: -0.23674 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.28158 HOMO: -7.01237 LUMO: 2.01092 factor:1 | 1 (-0.82725) | -1 | -1 |
| G: -5312.08863 HOMO: -6.61509 LUMO: -0.23674 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.62134 HOMO: -6.93618 LUMO: 1.63540 factor:1 | 1 (-1.16701) | -1 | -1 |
| G: -5312.08863 HOMO: -6.61509 LUMO: -0.23674 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.47763 HOMO: -6.98516 LUMO: 1.64629 factor:1 | 1 (-1.02331) | -1 | -1 |
| G: -5312.08863 HOMO: -6.61509 LUMO: -0.23674 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.59516 HOMO: -6.80285 LUMO: 1.95106 factor:1 | 1 (-1.14084) | -1 | -1 |
| G: -5312.08863 HOMO: -6.61509 LUMO: -0.23674 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11578.21272 HOMO: -6.76747 LUMO: 1.88303 factor:1 | 1 (-1.75840) | -1 | -1 |
| G: -5312.08863 HOMO: -6.61509 LUMO: -0.23674 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11578.00401 HOMO: -6.64230 LUMO: 1.90480 factor:1 | 1 (-1.54969) | -1 | -1 |
| G: -5312.08863 HOMO: -6.61509 LUMO: -0.23674 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11578.02303 HOMO: -6.93618 LUMO: 2.19324 factor:1 | 1 (-1.56871) | -1 | -1 |
| G: -5312.08863 HOMO: -6.61509 LUMO: -0.23674 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11578.83529 HOMO: -6.95523 LUMO: 1.80684 factor:1 | 1 (-2.38097) | -1 | -1 |
| G: -5312.08863 HOMO: -6.61509 LUMO: -0.23674 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11578.98079 HOMO: -6.66135 LUMO: 1.72792 factor:1 | 1 (-2.52647) | -1 | -1 |
| G: -5312.08863 HOMO: -6.61509 LUMO: -0.23674 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.97506 HOMO: -6.36202 LUMO: 1.89391 factor:1 | 1 (-1.52074) | -1 | -1 |
| G: -5312.08863 HOMO: -6.61509 LUMO: -0.23674 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11578.15620 HOMO: -7.03959 LUMO: 2.06262 factor:1 | 1 (-1.70188) | -1 | -1 |
| G: -5312.08863 HOMO: -6.61509 LUMO: -0.23674 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.79141 HOMO: -7.08584 LUMO: 2.01092 factor:1 | 1 (-1.33709) | 1 | -1 |
| G: -5312.08863 HOMO: -6.80285 LUMO: -0.55783 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11578.04156 HOMO: -6.96067 LUMO: 1.59731 factor:1 | 1 (-1.58724) | -1 | -1 |
| G: -5312.08863 HOMO: -6.80285 LUMO: -0.55783 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.78665 HOMO: -6.91169 LUMO: 1.37145 factor:1 | 1 (-1.33232) | -1 | -1 |
| G: -5312.08863 HOMO: -6.80285 LUMO: -0.55783 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.80286 HOMO: -6.94707 LUMO: 1.73064 factor:1 | 1 (-1.34854) | -1 | -1 |
| G: -5312.08863 HOMO: -6.80285 LUMO: -0.55783 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.73818 HOMO: -7.02326 LUMO: 1.41227 factor:1 | 1 (-1.28386) | -1 | -1 |
| G: -5312.08863 HOMO: -6.80285 LUMO: -0.55783 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.59813 HOMO: -6.72121 LUMO: 1.43132 factor:1 | 1 (-1.14380) | -1 | -1 |
| G: -5312.08863 HOMO: -6.80285 LUMO: -0.55783 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.75245 HOMO: -6.51168 LUMO: 1.72520 factor:1 | 1 (-0.29813) | -1 | -1 |
| G: -5312.08863 HOMO: -6.80285 LUMO: -0.55783 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.96494 HOMO: -6.98516 LUMO: 1.92929 factor:1 | 1 (-0.51062) | -1 | -1 |
| G: -5312.08863 HOMO: -6.80285 LUMO: -0.55783 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.84187 HOMO: -6.92802 LUMO: 2.07895 factor:1 | 1 (-0.38754) | -1 | -1 |
| G: -5312.08863 HOMO: -6.80285 LUMO: -0.55783 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.90619 HOMO: -7.02326 LUMO: 1.86398 factor:1 | 1 (-0.45187) | -1 | -1 |
| G: -5312.08863 HOMO: -6.80285 LUMO: -0.55783 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.92399 HOMO: -6.82462 LUMO: 1.86670 factor:1 | 1 (-0.46967) | -1 | -1 |
| G: -5312.08863 HOMO: -6.80285 LUMO: -0.55783 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.91158 HOMO: -6.83278 LUMO: 1.71160 factor:1 | 1 (-0.45726) | -1 | -1 |
| G: -5312.08863 HOMO: -6.80285 LUMO: -0.55783 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.82829 HOMO: -6.62869 LUMO: 1.69527 factor:1 | 1 (-0.37397) | -1 | -1 |
| G: -5312.08863 HOMO: -6.80285 LUMO: -0.55783 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.77049 HOMO: -6.84094 LUMO: 1.27349 factor:1 | 1 (-0.31617) | -1 | -1 |
| G: -5312.08863 HOMO: -6.80285 LUMO: -0.55783 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.73539 HOMO: -7.07768 LUMO: 1.27621 factor:1 | 1 (-0.28107) | 1 | -1 |
| G: -5312.08863 HOMO: -6.80285 LUMO: -0.55783 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.56192 HOMO: -7.06135 LUMO: 1.55105 factor:1 | 1 (-0.10759) | 1 | -1 |
| G: -5312.08863 HOMO: -6.80285 LUMO: -0.55783 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.92170 HOMO: -6.94162 LUMO: 1.64629 factor:1 | 1 (-0.46738) | -1 | -1 |
| G: -5312.08863 HOMO: -6.80285 LUMO: -0.55783 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.75297 HOMO: -7.07224 LUMO: 1.65445 factor:1 | 1 (-0.29864) | 1 | -1 |
| G: -5312.08863 HOMO: -6.80285 LUMO: -0.55783 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.69699 HOMO: -6.68584 LUMO: 1.91296 factor:1 | 1 (-0.24267) | -1 | -1 |
| G: -5312.08863 HOMO: -6.80285 LUMO: -0.55783 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.98160 HOMO: -7.09129 LUMO: 1.73609 factor:1 | 1 (-0.52728) | 1 | -1 |
| G: -5312.08863 HOMO: -6.80285 LUMO: -0.55783 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.72401 HOMO: -7.01237 LUMO: 2.01092 factor:1 | 1 (-0.26969) | -1 | -1 |
| G: -5312.08863 HOMO: -6.80285 LUMO: -0.55783 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.75727 HOMO: -6.93618 LUMO: 1.63540 factor:1 | 1 (-0.30294) | -1 | -1 |
| G: -5312.08863 HOMO: -6.80285 LUMO: -0.55783 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.85528 HOMO: -6.98516 LUMO: 1.64629 factor:1 | 1 (-0.40096) | -1 | -1 |
| G: -5312.08863 HOMO: -6.80285 LUMO: -0.55783 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.76763 HOMO: -6.80285 LUMO: 1.95106 factor:1 | 1 (-0.31331) | -1 | -1 |
| G: -5312.08863 HOMO: -6.80285 LUMO: -0.55783 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.92845 HOMO: -6.76747 LUMO: 1.88303 factor:1 | 1 (-0.47413) | -1 | -1 |
| G: -5312.08863 HOMO: -6.80285 LUMO: -0.55783 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.62467 HOMO: -6.64230 LUMO: 1.90480 factor:1 | 1 (-0.17034) | -1 | -1 |
| G: -5312.08863 HOMO: -6.80285 LUMO: -0.55783 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.77778 HOMO: -6.93618 LUMO: 2.19324 factor:1 | 1 (-0.32346) | -1 | -1 |
| G: -5312.08863 HOMO: -6.80285 LUMO: -0.55783 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.50012 HOMO: -6.95523 LUMO: 1.80684 factor:1 | 1 (-0.04580) | -1 | -1 |
| G: -5312.08863 HOMO: -6.80285 LUMO: -0.55783 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.82051 HOMO: -6.66135 LUMO: 1.72792 factor:1 | 1 (-0.36618) | -1 | -1 |
| G: -5312.08863 HOMO: -6.80285 LUMO: -0.55783 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.71103 HOMO: -6.36202 LUMO: 1.89391 factor:1 | 1 (-0.25671) | -1 | -1 |
| G: -5312.08863 HOMO: -6.80285 LUMO: -0.55783 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.78891 HOMO: -7.03959 LUMO: 2.06262 factor:1 | 1 (-0.33459) | -1 | -1 |
| G: -5312.08863 HOMO: -6.80285 LUMO: -0.55783 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.69014 HOMO: -7.08584 LUMO: 2.01092 factor:1 | 1 (-0.23581) | 1 | -1 |
| G: -5312.08863 HOMO: -7.16476 LUMO: 2.86264 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.82894 HOMO: -6.96067 LUMO: 1.59731 factor:1 | 1 (-0.37462) | -1 | -1 |
| G: -5312.08863 HOMO: -7.16476 LUMO: 2.86264 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.67944 HOMO: -6.91169 LUMO: 1.37145 factor:1 | 1 (-0.22512) | -1 | -1 |
| G: -5312.08863 HOMO: -7.16476 LUMO: 2.86264 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.68910 HOMO: -6.94707 LUMO: 1.73064 factor:1 | 1 (-0.23478) | -1 | -1 |
| G: -5312.08863 HOMO: -7.16476 LUMO: 2.86264 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.54450 HOMO: -7.02326 LUMO: 1.41227 factor:1 | 1 (-0.09018) | -1 | -1 |
| G: -5312.08863 HOMO: -7.16476 LUMO: 2.86264 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.59109 HOMO: -6.72121 LUMO: 1.43132 factor:1 | 1 (-0.13676) | -1 | -1 |
| G: -5312.08863 HOMO: -7.16476 LUMO: 2.86264 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.88883 HOMO: -6.51168 LUMO: 1.72520 factor:1 | 1 (-0.43451) | -1 | -1 |
| G: -5312.08863 HOMO: -7.16476 LUMO: 2.86264 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.73686 HOMO: -6.98516 LUMO: 1.92929 factor:1 | 1 (-0.28254) | -1 | -1 |
| G: -5312.08863 HOMO: -7.16476 LUMO: 2.86264 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.79438 HOMO: -6.92802 LUMO: 2.07895 factor:1 | 1 (-0.34006) | -1 | -1 |
| G: -5312.08863 HOMO: -7.16476 LUMO: 2.86264 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.79302 HOMO: -7.02326 LUMO: 1.86398 factor:1 | 1 (-0.33870) | -1 | -1 |
| G: -5312.08863 HOMO: -7.16476 LUMO: 2.86264 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11578.18801 HOMO: -6.82462 LUMO: 1.86670 factor:1 | 1 (-1.73369) | -1 | -1 |
| G: -5312.08863 HOMO: -7.16476 LUMO: 2.86264 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11578.97167 HOMO: -6.83278 LUMO: 1.71160 factor:1 | 1 (-2.51735) | -1 | -1 |
| G: -5312.08863 HOMO: -7.16476 LUMO: 2.86264 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.98662 HOMO: -6.62869 LUMO: 1.69527 factor:1 | 1 (-1.53230) | -1 | -1 |
| G: -5312.08863 HOMO: -7.16476 LUMO: 2.86264 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11578.13373 HOMO: -6.84094 LUMO: 1.27349 factor:1 | 1 (-1.67941) | -1 | -1 |
| G: -5312.08863 HOMO: -7.16476 LUMO: 2.86264 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11578.14733 HOMO: -7.07768 LUMO: 1.27621 factor:1 | 1 (-1.69301) | -1 | -1 |
| G: -5312.08863 HOMO: -7.16476 LUMO: 2.86264 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11578.00404 HOMO: -7.06135 LUMO: 1.55105 factor:1 | 1 (-1.54972) | -1 | -1 |
| G: -5312.08863 HOMO: -7.16476 LUMO: 2.86264 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.68978 HOMO: -6.94162 LUMO: 1.64629 factor:1 | 1 (-0.23546) | -1 | -1 |
| G: -5312.08863 HOMO: -7.16476 LUMO: 2.86264 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.74864 HOMO: -7.07224 LUMO: 1.65445 factor:1 | 1 (-0.29432) | -1 | -1 |
| G: -5312.08863 HOMO: -7.16476 LUMO: 2.86264 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.75269 HOMO: -6.68584 LUMO: 1.91296 factor:1 | 1 (-0.29837) | -1 | -1 |
| G: -5312.08863 HOMO: -7.16476 LUMO: 2.86264 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.55775 HOMO: -7.09129 LUMO: 1.73609 factor:1 | 1 (-0.10343) | -1 | -1 |
| G: -5312.08863 HOMO: -7.16476 LUMO: 2.86264 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.61917 HOMO: -7.01237 LUMO: 2.01092 factor:1 | 1 (-0.16485) | -1 | -1 |
| G: -5312.08863 HOMO: -7.16476 LUMO: 2.86264 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.43552 HOMO: -6.93618 LUMO: 1.63540 factor:1 | -1 (0.01880) | -1 | -1 |
| G: -5312.08863 HOMO: -7.16476 LUMO: 2.86264 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.42877 HOMO: -6.98516 LUMO: 1.64629 factor:1 | -1 (0.02555) | -1 | -1 |
| G: -5312.08863 HOMO: -7.16476 LUMO: 2.86264 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.81506 HOMO: -6.80285 LUMO: 1.95106 factor:1 | 1 (-0.36074) | -1 | -1 |
| G: -5312.08863 HOMO: -7.16476 LUMO: 2.86264 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.65373 HOMO: -6.76747 LUMO: 1.88303 factor:1 | 1 (-0.19941) | -1 | -1 |
| G: -5312.08863 HOMO: -7.16476 LUMO: 2.86264 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.64442 HOMO: -6.64230 LUMO: 1.90480 factor:1 | 1 (-0.19010) | -1 | -1 |
| G: -5312.08863 HOMO: -7.16476 LUMO: 2.86264 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.74826 HOMO: -6.93618 LUMO: 2.19324 factor:1 | 1 (-0.29394) | -1 | -1 |
| G: -5312.08863 HOMO: -7.16476 LUMO: 2.86264 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11578.46035 HOMO: -6.95523 LUMO: 1.80684 factor:1 | 1 (-2.00602) | -1 | -1 |
| G: -5312.08863 HOMO: -7.16476 LUMO: 2.86264 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.67075 HOMO: -6.66135 LUMO: 1.72792 factor:1 | 1 (-1.21643) | -1 | -1 |
| G: -5312.08863 HOMO: -7.16476 LUMO: 2.86264 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.71456 HOMO: -6.36202 LUMO: 1.89391 factor:1 | 1 (-1.26024) | -1 | -1 |
| G: -5312.08863 HOMO: -7.16476 LUMO: 2.86264 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.74607 HOMO: -7.03959 LUMO: 2.06262 factor:1 | 1 (-1.29175) | -1 | -1 |
| G: -5312.08863 HOMO: -7.16476 LUMO: 2.86264 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.74722 HOMO: -7.08584 LUMO: 2.01092 factor:1 | 1 (-1.29289) | -1 | -1 |
| G: -5312.08863 HOMO: -6.50352 LUMO: 2.10888 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.60368 HOMO: -6.96067 LUMO: 1.59731 factor:1 | 1 (-1.14935) | 1 | 1 |
| G: -5312.08863 HOMO: -6.50352 LUMO: 2.10888 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.80047 HOMO: -6.91169 LUMO: 1.37145 factor:1 | 1 (-1.34615) | -1 | -1 |
| G: -5311.25950 HOMO: -6.50352 LUMO: 2.10888 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.03352 HOMO: -6.94707 LUMO: 1.73064 factor:1 | 1 (-1.40833) | 1 | 1 |
| G: -5311.25950 HOMO: -6.50352 LUMO: 2.10888 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.84902 HOMO: -7.02326 LUMO: 1.41227 factor:1 | 1 (-1.22383) | -1 | -1 |
| G: -5311.25950 HOMO: -6.50352 LUMO: 2.10888 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.57944 HOMO: -6.72121 LUMO: 1.43132 factor:1 | 1 (-0.95425) | -1 | -1 |
| G: -5311.25950 HOMO: -6.50352 LUMO: 2.10888 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11578.44220 HOMO: -6.51168 LUMO: 1.72520 factor:1 | 1 (-2.81700) | 1 | 1 |
| G: -5311.25950 HOMO: -6.50352 LUMO: 2.10888 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11578.06807 HOMO: -6.98516 LUMO: 1.92929 factor:1 | 1 (-2.44287) | 1 | 1 |
| G: -5311.25950 HOMO: -6.50352 LUMO: 2.10888 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11579.01581 HOMO: -6.92802 LUMO: 2.07895 factor:1 | 1 (-3.39062) | 1 | 1 |
| G: -5311.25950 HOMO: -6.50352 LUMO: 2.10888 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11578.14426 HOMO: -7.02326 LUMO: 1.86398 factor:1 | 1 (-2.51907) | 1 | 1 |
| G: -5311.25950 HOMO: -6.50352 LUMO: 2.10888 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11578.29803 HOMO: -6.82462 LUMO: 1.86670 factor:1 | 1 (-2.67284) | 1 | 1 |
| G: -5311.25950 HOMO: -6.50352 LUMO: 2.10888 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.87095 HOMO: -6.83278 LUMO: 1.71160 factor:1 | 1 (-2.24576) | 1 | 1 |
| G: -5311.25950 HOMO: -6.50352 LUMO: 2.10888 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.91870 HOMO: -6.62869 LUMO: 1.69527 factor:1 | 1 (-2.29351) | 1 | 1 |
| G: -5311.25950 HOMO: -6.50352 LUMO: 2.10888 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.90734 HOMO: -6.84094 LUMO: 1.27349 factor:1 | 1 (-1.28215) | -1 | -1 |
| G: -5311.25950 HOMO: -6.50352 LUMO: 2.10888 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.31279 HOMO: -7.07768 LUMO: 1.27621 factor:1 | 1 (-1.68760) | -1 | -1 |
| G: -5311.25950 HOMO: -6.50352 LUMO: 2.10888 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.94470 HOMO: -7.06135 LUMO: 1.55105 factor:1 | 1 (-1.31951) | -1 | -1 |
| G: -5311.25950 HOMO: -6.50352 LUMO: 2.10888 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.26729 HOMO: -6.94162 LUMO: 1.64629 factor:1 | 1 (-1.64210) | 1 | 1 |
| G: -5311.25950 HOMO: -6.50352 LUMO: 2.10888 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.20982 HOMO: -7.07224 LUMO: 1.65445 factor:1 | 1 (-1.58463) | 1 | 1 |
| G: -5311.25950 HOMO: -6.50352 LUMO: 2.10888 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.44933 HOMO: -6.68584 LUMO: 1.91296 factor:1 | 1 (-1.82414) | 1 | 1 |
| G: -5311.25950 HOMO: -6.50352 LUMO: 2.10888 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.61638 HOMO: -7.09129 LUMO: 1.73609 factor:1 | 1 (-1.99119) | 1 | 1 |
| G: -5311.25950 HOMO: -6.50352 LUMO: 2.10888 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.80545 HOMO: -7.01237 LUMO: 2.01092 factor:1 | 1 (-2.18026) | 1 | 1 |
| G: -5311.25950 HOMO: -6.50352 LUMO: 2.10888 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.94529 HOMO: -6.93618 LUMO: 1.63540 factor:1 | 1 (-2.32010) | 1 | 1 |
| G: -5311.25950 HOMO: -6.50352 LUMO: 2.10888 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.65973 HOMO: -6.98516 LUMO: 1.64629 factor:1 | 1 (-2.03454) | 1 | 1 |
| G: -5311.25950 HOMO: -6.50352 LUMO: 2.10888 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.23591 HOMO: -6.80285 LUMO: 1.95106 factor:1 | 1 (-1.61072) | 1 | 1 |
| G: -5311.25950 HOMO: -6.50352 LUMO: 2.10888 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.16650 HOMO: -6.76747 LUMO: 1.88303 factor:1 | 1 (-1.54131) | 1 | 1 |
| G: -5311.25950 HOMO: -6.50352 LUMO: 2.10888 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.81999 HOMO: -6.64230 LUMO: 1.90480 factor:1 | 1 (-1.19480) | 1 | 1 |
| G: -5311.25950 HOMO: -6.50352 LUMO: 2.10888 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.19684 HOMO: -6.93618 LUMO: 2.19324 factor:1 | 1 (-1.57165) | 1 | 1 |
| G: -5311.25950 HOMO: -6.50352 LUMO: 2.10888 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.95011 HOMO: -6.95523 LUMO: 1.80684 factor:1 | 1 (-1.32492) | 1 | 1 |
| G: -5311.25950 HOMO: -6.50352 LUMO: 2.10888 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.75980 HOMO: -6.66135 LUMO: 1.72792 factor:1 | 1 (-1.13461) | 1 | 1 |
| G: -5311.25950 HOMO: -6.50352 LUMO: 2.10888 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.04078 HOMO: -6.36202 LUMO: 1.89391 factor:1 | 1 (-1.41559) | -1 | -1 |
| G: -5311.25950 HOMO: -6.50352 LUMO: 2.10888 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.98805 HOMO: -7.03959 LUMO: 2.06262 factor:1 | 1 (-1.36286) | 1 | 1 |
| G: -5311.25950 HOMO: -6.50352 LUMO: 2.10888 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11578.40693 HOMO: -7.08584 LUMO: 2.01092 factor:1 | 1 (-2.78174) | 1 | 1 |
| G: -5311.25950 HOMO: -6.59604 LUMO: 2.33746 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.71807 HOMO: -6.96067 LUMO: 1.59731 factor:1 | 1 (-2.09288) | 1 | 1 |
| G: -5311.25950 HOMO: -6.59604 LUMO: 2.33746 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.81658 HOMO: -6.91169 LUMO: 1.37145 factor:1 | 1 (-2.19139) | -1 | -1 |
| G: -5311.25950 HOMO: -6.59604 LUMO: 2.33746 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11578.02926 HOMO: -6.94707 LUMO: 1.73064 factor:1 | 1 (-2.40407) | 1 | 1 |
| G: -5311.25950 HOMO: -6.59604 LUMO: 2.33746 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11578.34372 HOMO: -7.02326 LUMO: 1.41227 factor:1 | 1 (-2.71853) | -1 | -1 |
| G: -5311.25950 HOMO: -6.59604 LUMO: 2.33746 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11578.21977 HOMO: -6.72121 LUMO: 1.43132 factor:1 | 1 (-2.59458) | -1 | -1 |
| G: -5311.25950 HOMO: -6.59604 LUMO: 2.33746 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11578.26497 HOMO: -6.51168 LUMO: 1.72520 factor:1 | 1 (-2.63978) | -1 | -1 |
| G: -5311.25950 HOMO: -6.59604 LUMO: 2.33746 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11578.14668 HOMO: -6.98516 LUMO: 1.92929 factor:1 | 1 (-2.52149) | 1 | 1 |
| G: -5311.25950 HOMO: -6.59604 LUMO: 2.33746 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.03763 HOMO: -6.92802 LUMO: 2.07895 factor:1 | 1 (-1.41243) | 1 | 1 |
| G: -5311.25950 HOMO: -6.59604 LUMO: 2.33746 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.87120 HOMO: -7.02326 LUMO: 1.86398 factor:1 | 1 (-1.24601) | 1 | 1 |
| G: -5311.25950 HOMO: -6.59604 LUMO: 2.33746 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.07972 HOMO: -6.82462 LUMO: 1.86670 factor:1 | 1 (-1.45453) | 1 | 1 |
| G: -5311.25950 HOMO: -6.59604 LUMO: 2.33746 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11578.43659 HOMO: -6.83278 LUMO: 1.71160 factor:1 | 1 (-2.81140) | 1 | 1 |
| G: -5311.25950 HOMO: -6.59604 LUMO: 2.33746 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.90921 HOMO: -6.62869 LUMO: 1.69527 factor:1 | 1 (-2.28401) | 1 | 1 |
| G: -5311.25950 HOMO: -6.59604 LUMO: 2.33746 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.80221 HOMO: -6.84094 LUMO: 1.27349 factor:1 | 1 (-2.17702) | -1 | -1 |
| G: -5311.25950 HOMO: -6.59604 LUMO: 2.33746 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.90619 HOMO: -7.07768 LUMO: 1.27621 factor:1 | 1 (-2.28099) | -1 | -1 |
| G: -5311.25950 HOMO: -6.59604 LUMO: 2.33746 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11578.00703 HOMO: -7.06135 LUMO: 1.55105 factor:1 | 1 (-2.38184) | -1 | -1 |
| G: -5311.25950 HOMO: -6.59604 LUMO: 2.33746 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.87946 HOMO: -6.94162 LUMO: 1.64629 factor:1 | 1 (-2.25427) | 1 | 1 |
| G: -5311.25950 HOMO: -6.59604 LUMO: 2.33746 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.13657 HOMO: -7.07224 LUMO: 1.65445 factor:1 | 1 (-1.51137) | 1 | 1 |
| G: -5311.25950 HOMO: -6.59604 LUMO: 2.33746 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.05120 HOMO: -6.68584 LUMO: 1.91296 factor:1 | 1 (-1.42601) | 1 | 1 |
| G: -5311.25950 HOMO: -6.59604 LUMO: 2.33746 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.94410 HOMO: -7.09129 LUMO: 1.73609 factor:1 | 1 (-1.31891) | 1 | 1 |
| G: -5311.25950 HOMO: -6.59604 LUMO: 2.33746 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.12138 HOMO: -7.01237 LUMO: 2.01092 factor:1 | 1 (-1.49619) | 1 | 1 |
| G: -5311.25950 HOMO: -6.59604 LUMO: 2.33746 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.04282 HOMO: -6.93618 LUMO: 1.63540 factor:1 | 1 (-1.41763) | 1 | 1 |
| G: -5311.25950 HOMO: -6.59604 LUMO: 2.33746 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.03874 HOMO: -6.98516 LUMO: 1.64629 factor:1 | 1 (-1.41355) | 1 | 1 |
| G: -5311.25950 HOMO: -6.59604 LUMO: 2.33746 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.05523 HOMO: -6.80285 LUMO: 1.95106 factor:1 | 1 (-1.43004) | 1 | 1 |
| G: -5311.25950 HOMO: -6.59604 LUMO: 2.33746 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.92949 HOMO: -6.76747 LUMO: 1.88303 factor:1 | 1 (-1.30430) | 1 | 1 |
| G: -5311.25950 HOMO: -6.59604 LUMO: 2.33746 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.12590 HOMO: -6.64230 LUMO: 1.90480 factor:1 | 1 (-1.50071) | 1 | 1 |
| G: -5311.25950 HOMO: -6.59604 LUMO: 2.33746 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.08603 HOMO: -6.93618 LUMO: 2.19324 factor:1 | 1 (-1.46084) | 1 | 1 |
| G: -5311.25950 HOMO: -6.59604 LUMO: 2.33746 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.07700 HOMO: -6.95523 LUMO: 1.80684 factor:1 | 1 (-1.45181) | 1 | 1 |
| G: -5311.25950 HOMO: -6.59604 LUMO: 2.33746 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.84032 HOMO: -6.66135 LUMO: 1.72792 factor:1 | 1 (-1.21512) | 1 | 1 |
| G: -5311.25950 HOMO: -6.59604 LUMO: 2.33746 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.02666 HOMO: -6.36202 LUMO: 1.89391 factor:1 | 1 (-1.40147) | -1 | -1 |
| G: -5311.25950 HOMO: -6.59604 LUMO: 2.33746 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.85101 HOMO: -7.03959 LUMO: 2.06262 factor:1 | 1 (-1.22582) | 1 | 1 |
| G: -5311.25950 HOMO: -6.59604 LUMO: 2.33746 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.06329 HOMO: -7.08584 LUMO: 2.01092 factor:1 | 1 (-1.43809) | 1 | 1 |
| G: -5311.25950 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11579.05184 HOMO: -7.06135 LUMO: 0.75376 factor:1 | 1 (-3.42665) | 1 | -1 |
| G: -5311.25950 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11578.24889 HOMO: -5.10213 LUMO: 0.77825 factor:1 | 1 (-2.62369) | -1 | -1 |
| G: -5311.25950 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11578.30391 HOMO: -5.84228 LUMO: 0.50341 factor:1 | 1 (-2.67872) | -1 | -1 |
| G: -5311.25950 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.91966 HOMO: -5.39874 LUMO: 0.68028 factor:1 | 1 (-1.29447) | -1 | -1 |
| G: -5311.25950 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.90990 HOMO: -5.16744 LUMO: 1.14832 factor:1 | 1 (-1.28470) | -1 | -1 |
| G: -5311.25950 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.92821 HOMO: -5.80963 LUMO: 0.35647 factor:1 | 1 (-1.30302) | -1 | -1 |
| G: -5311.25950 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.01300 HOMO: -5.02322 LUMO: 1.07213 factor:1 | 1 (-1.38781) | -1 | -1 |
| G: -5311.25950 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11578.36530 HOMO: -5.80963 LUMO: 0.56328 factor:1 | 1 (-2.74010) | -1 | -1 |
| G: -5311.25950 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.72863 HOMO: -5.45316 LUMO: 0.78369 factor:1 | 1 (-2.10344) | -1 | -1 |
| G: -5311.25950 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.93634 HOMO: -5.25452 LUMO: 0.82178 factor:1 | 1 (-2.31114) | -1 | -1 |
| G: -5311.25950 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.90281 HOMO: -5.21370 LUMO: 1.03947 factor:1 | 1 (-2.27762) | -1 | -1 |
| G: -5311.25950 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.89751 HOMO: -6.04365 LUMO: 0.31837 factor:1 | 1 (-2.27231) | -1 | -1 |
| G: -5311.25950 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.93692 HOMO: -5.86405 LUMO: 0.55511 factor:1 | 1 (-1.31172) | -1 | -1 |
| G: -5311.25950 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.06900 HOMO: -5.64908 LUMO: 0.71022 factor:1 | 1 (-1.44381) | -1 | -1 |
| G: -5311.25950 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.92396 HOMO: -5.94297 LUMO: 0.68301 factor:1 | 1 (-1.29877) | -1 | -1 |
| G: -5311.25950 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.15140 HOMO: -6.01916 LUMO: 0.56328 factor:1 | 1 (-1.52621) | -1 | -1 |
| G: -5311.25950 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.18797 HOMO: -6.05181 LUMO: 0.35103 factor:1 | 1 (-1.56278) | -1 | -1 |
| G: -5311.25950 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.46615 HOMO: -6.08447 LUMO: 0.48436 factor:1 | 1 (-1.84096) | -1 | -1 |
| G: -5311.25950 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.13589 HOMO: -5.86950 LUMO: 0.36735 factor:1 | 1 (-1.51069) | -1 | -1 |
| G: -5311.25950 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.33159 HOMO: -5.33615 LUMO: 0.65852 factor:1 | 1 (-1.70640) | -1 | -1 |
| G: -5311.25950 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.22342 HOMO: -5.36064 LUMO: 0.86804 factor:1 | 1 (-1.59823) | -1 | -1 |
| G: -5311.25950 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.13433 HOMO: -5.74160 LUMO: 0.64491 factor:1 | 1 (-1.50914) | -1 | -1 |
| G: -5311.25950 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.29834 HOMO: -5.23003 LUMO: 0.66124 factor:1 | 1 (-1.67315) | -1 | -1 |
| G: -5311.25950 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.22571 HOMO: -5.77698 LUMO: 0.84083 factor:1 | 1 (-1.60052) | -1 | -1 |
| G: -5311.25950 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.12233 HOMO: -5.60555 LUMO: 0.84355 factor:1 | 1 (-1.49714) | -1 | -1 |
| G: -5311.25950 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.17338 HOMO: -7.11578 LUMO: -1.62452 factor:1 | 1 (-1.54819) | -1 | -1 |
| G: -5311.25950 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.99752 HOMO: -7.23279 LUMO: -1.63813 factor:1 | 1 (-1.37232) | -1 | -1 |
| G: -5311.25950 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.02682 HOMO: -6.68312 LUMO: -0.88709 factor:1 | 1 (-1.40163) | -1 | -1 |
| G: -5311.25950 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.08987 HOMO: -6.99333 LUMO: -0.88709 factor:1 | 1 (-1.46468) | -1 | -1 |
| G: -5311.25950 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.17028 HOMO: -7.40694 LUMO: 0.11973 factor:1 | 1 (-1.54509) | 1 | 1 |
| G: -5311.25950 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.28193 HOMO: -6.74026 LUMO: -0.72927 factor:1 | 1 (-1.65674) | -1 | -1 |
| G: -5311.25950 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.68126 HOMO: -6.67223 LUMO: -0.70750 factor:1 | 1 (-2.05607) | -1 | -1 |
| G: -5311.25950 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.87073 HOMO: -7.06952 LUMO: -1.40139 factor:1 | 1 (-2.24554) | -1 | -1 |
| G: -5311.25950 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.64139 HOMO: -7.21374 LUMO: -1.13199 factor:1 | 1 (-2.01620) | -1 | -1 |
| G: -5311.25950 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.89272 HOMO: -6.54706 LUMO: -1.34424 factor:1 | 1 (-2.26752) | -1 | -1 |
| G: -5311.25950 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.62999 HOMO: -7.51851 LUMO: -1.05852 factor:1 | 1 (-2.00480) | -1 | -1 |
| G: -5311.25950 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.95459 HOMO: -7.07224 LUMO: -1.89391 factor:1 | 1 (-2.32940) | -1 | -1 |
| G: -5311.25950 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.05490 HOMO: -6.65863 LUMO: -0.46804 factor:1 | 1 (-1.42971) | -1 | -1 |
| G: -5311.25950 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.99806 HOMO: -7.24367 LUMO: 0.29388 factor:1 | 1 (-1.37287) | 1 | 1 |
| G: -5311.25950 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.06497 HOMO: -7.02326 LUMO: -0.87893 factor:1 | 1 (-1.43978) | -1 | -1 |
| G: -5311.25950 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.12217 HOMO: -6.88176 LUMO: 0.71566 factor:1 | 1 (-1.49698) | -1 | -1 |
| G: -5311.25950 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.08105 HOMO: -6.46543 LUMO: 1.01498 factor:1 | 1 (-1.45586) | -1 | -1 |
| G: -5311.25950 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.15738 HOMO: -6.30760 LUMO: 0.17687 factor:1 | 1 (-1.53219) | -1 | -1 |
| G: -5311.25950 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.20478 HOMO: -6.73210 LUMO: -1.06941 factor:1 | 1 (-1.57959) | -1 | -1 |
| G: -5311.25950 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.15923 HOMO: -6.83550 LUMO: -0.75920 factor:1 | 1 (-1.53404) | -1 | -1 |
| G: -5311.25950 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.50906 HOMO: -6.94707 LUMO: 0.42178 factor:1 | 1 (-1.88387) | -1 | -1 |
| G: -5311.25950 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.31507 HOMO: -6.77019 LUMO: -0.38096 factor:1 | 1 (-1.68988) | -1 | -1 |
| G: -5311.25950 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.22440 HOMO: -7.34163 LUMO: 0.35103 factor:1 | 1 (-1.59921) | 1 | 1 |
| G: -5311.25950 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.26255 HOMO: -6.87632 LUMO: -0.87349 factor:1 | 1 (-1.63736) | -1 | -1 |
| G: -5311.25950 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.25654 HOMO: -7.06952 LUMO: -1.47214 factor:1 | 1 (-1.63135) | -1 | -1 |
| G: -5311.25950 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.12729 HOMO: -6.58788 LUMO: -0.37824 factor:1 | 1 (-1.50210) | -1 | -1 |
| G: -5311.25950 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.22789 HOMO: -6.92802 LUMO: -1.24900 factor:1 | 1 (-1.60270) | -1 | -1 |
| G: -5311.25950 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.18367 HOMO: -7.01237 LUMO: -1.31975 factor:1 | 1 (-1.55848) | -1 | -1 |
| G: -5311.25950 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.06089 HOMO: -6.74842 LUMO: 0.45987 factor:1 | 1 (-1.43570) | -1 | -1 |
| G: -5311.25950 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.70915 HOMO: -6.53890 LUMO: 0.94424 factor:1 | 1 (-2.08396) | -1 | -1 |
| G: -5311.25950 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.97250 HOMO: -6.52257 LUMO: -0.66940 factor:1 | 1 (-2.34731) | -1 | -1 |
| G: -5311.25950 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.98733 HOMO: -6.56883 LUMO: -1.48302 factor:1 | 1 (-2.36214) | -1 | -1 |
| G: -5311.25950 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.89506 HOMO: -7.21646 LUMO: 0.13061 factor:1 | 1 (-2.26986) | 1 | 1 |
| G: -5311.25950 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11578.00728 HOMO: -6.62597 LUMO: -0.64763 factor:1 | 1 (-2.38208) | -1 | -1 |
| G: -5311.25950 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.81571 HOMO: -7.38789 LUMO: 0.31021 factor:1 | 1 (-2.19052) | 1 | 1 |
| G: -5311.25950 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.80836 HOMO: -6.74570 LUMO: -0.70750 factor:1 | 1 (-2.18317) | -1 | -1 |
| G: -5311.25950 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.17161 HOMO: -6.95251 LUMO: -1.25989 factor:1 | 1 (-1.54642) | -1 | -1 |
| G: -5311.25950 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.31047 HOMO: -7.13483 LUMO: -0.76736 factor:1 | 1 (-1.68528) | -1 | -1 |
| G: -5311.25950 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.22168 HOMO: -6.93618 LUMO: -1.24628 factor:1 | 1 (-1.59649) | -1 | -1 |
| G: -5311.25950 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.13526 HOMO: -7.03686 LUMO: 0.26395 factor:1 | 1 (-1.51007) | -1 | -1 |
| G: -5311.25950 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.58749 HOMO: -6.52257 LUMO: -0.84355 factor:1 | 1 (-1.96229) | -1 | -1 |
| G: -5311.25950 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.71002 HOMO: -6.83278 LUMO: -0.49525 factor:1 | 1 (-2.08483) | -1 | -1 |
| G: -5311.25950 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.74716 HOMO: -7.18381 LUMO: -1.64629 factor:1 | 1 (-2.12197) | -1 | -1 |
| G: -5311.25950 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.88082 HOMO: -6.74842 LUMO: -0.81090 factor:1 | 1 (-2.25563) | -1 | -1 |
| G: -5311.25950 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.70433 HOMO: -7.09401 LUMO: -0.92519 factor:1 | 1 (-2.07914) | -1 | -1 |
| G: -5311.25950 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.57698 HOMO: -7.20285 LUMO: -0.81634 factor:1 | 1 (-1.95179) | -1 | -1 |
| G: -5311.25950 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.69598 HOMO: -6.72665 LUMO: 0.77008 factor:1 | 1 (-2.07079) | -1 | -1 |
| G: -5311.25950 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.75065 HOMO: -6.80829 LUMO: 0.86532 factor:1 | 1 (-2.12545) | -1 | -1 |
| G: -5311.25950 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.51976 HOMO: -6.20964 LUMO: 0.99866 factor:1 | 1 (-1.89457) | -1 | -1 |
| G: -5311.25950 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.58476 HOMO: -6.52801 LUMO: 1.07757 factor:1 | 1 (-1.95957) | -1 | -1 |
| G: -5311.25950 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.88763 HOMO: -6.74298 LUMO: -0.67756 factor:1 | 1 (-2.26244) | -1 | -1 |
| G: -5311.25950 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.91780 HOMO: -7.43959 LUMO: 0.03265 factor:1 | 1 (-2.29261) | 1 | 1 |
| G: -5311.25950 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.67233 HOMO: -6.46815 LUMO: -0.29933 factor:1 | 1 (-2.04714) | -1 | -1 |
| G: -5311.25950 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.71426 HOMO: -6.70489 LUMO: -0.97145 factor:1 | 1 (-2.08907) | -1 | -1 |
| G: -5311.25950 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11578.38712 HOMO: -6.30216 LUMO: -1.39322 factor:1 | 1 (-2.76193) | -1 | -1 |
| G: -5311.25950 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11579.11660 HOMO: -7.01782 LUMO: -1.07485 factor:1 | 1 (-3.49141) | -1 | -1 |
| G: -5311.25950 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11578.42862 HOMO: -6.93074 LUMO: 0.25851 factor:1 | 1 (-2.80343) | -1 | -1 |
| G: -5311.25950 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.91500 HOMO: -7.07224 LUMO: 0.09524 factor:1 | 1 (-2.28981) | 1 | 1 |
| G: -5311.25950 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.91029 HOMO: -6.62325 LUMO: -0.45443 factor:1 | 1 (-2.28510) | -1 | -1 |
| G: -5311.25950 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11578.02831 HOMO: -7.09945 LUMO: -1.20274 factor:1 | 1 (-2.40312) | -1 | -1 |
| G: -5311.25950 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11578.37950 HOMO: -6.56067 LUMO: -1.39322 factor:1 | 1 (-2.75431) | -1 | -1 |
| G: -5311.25950 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11578.22298 HOMO: -6.75387 LUMO: -0.72654 factor:1 | 1 (-2.59779) | -1 | -1 |
| G: -5311.25950 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11578.33262 HOMO: -6.28583 LUMO: -2.35651 factor:1 | 1 (-2.70742) | -1 | -1 |
| G: -5311.25950 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.01199 HOMO: -6.55522 LUMO: -1.33608 factor:1 | 1 (-1.38680) | -1 | -1 |
| G: -5311.25950 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.90432 HOMO: -7.19741 LUMO: -0.93607 factor:1 | 1 (-1.27913) | -1 | -1 |
| G: -5311.25950 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.92502 HOMO: -6.39740 LUMO: -1.14832 factor:1 | 1 (-1.29983) | -1 | -1 |
| G: -5311.25950 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.15861 HOMO: -7.11850 LUMO: -0.97417 factor:1 | 1 (-1.53342) | -1 | -1 |
| G: -5311.25950 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11578.59148 HOMO: -6.57699 LUMO: -1.14016 factor:1 | 1 (-2.96629) | -1 | -1 |
| G: -5311.25950 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.94219 HOMO: -6.57699 LUMO: -1.31975 factor:1 | 1 (-2.31700) | -1 | -1 |
| G: -5311.25950 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.91201 HOMO: -6.69128 LUMO: -0.76736 factor:1 | 1 (-2.28682) | -1 | -1 |
| G: -5311.25950 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.96205 HOMO: -7.25728 LUMO: 0.29660 factor:1 | 1 (-2.33686) | 1 | 1 |
| G: -5311.25950 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.99577 HOMO: -6.37019 LUMO: -0.95240 factor:1 | 1 (-1.37058) | -1 | -1 |
| G: -5311.25950 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.90045 HOMO: -6.48447 LUMO: -0.55511 factor:1 | 1 (-1.27526) | -1 | -1 |
| G: -5311.25950 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.05071 HOMO: -6.37291 LUMO: -0.78641 factor:1 | 1 (-1.42552) | -1 | -1 |
| G: -5311.25950 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.38057 HOMO: -6.65863 LUMO: -0.69933 factor:1 | 1 (-1.75538) | -1 | -1 |
| G: -5311.25950 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.16176 HOMO: -6.44638 LUMO: -0.16055 factor:1 | 1 (-1.53657) | -1 | -1 |
| G: -5311.25950 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.94481 HOMO: -6.41917 LUMO: -0.20136 factor:1 | 1 (-1.31962) | -1 | -1 |
| G: -5311.25950 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.86679 HOMO: -7.33347 LUMO: 0.12789 factor:1 | 1 (-1.24160) | 1 | 1 |
| G: -5311.25950 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.16906 HOMO: -6.70489 LUMO: -0.52518 factor:1 | 1 (-1.54387) | -1 | -1 |
| G: -5311.25950 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.93460 HOMO: -7.25183 LUMO: 0.32109 factor:1 | 1 (-1.30941) | 1 | 1 |
| G: -5311.25950 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.21706 HOMO: -7.29265 LUMO: 0.28028 factor:1 | 1 (-1.59187) | 1 | 1 |
| G: -5311.25950 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.88181 HOMO: -6.57155 LUMO: -0.51702 factor:1 | 1 (-1.25662) | -1 | -1 |
| G: -5311.25950 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.90274 HOMO: -7.08040 LUMO: 0.39729 factor:1 | 1 (-1.27755) | 1 | 1 |
| G: -5311.25950 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.03129 HOMO: -6.24501 LUMO: -0.44627 factor:1 | 1 (-1.40609) | -1 | -1 |
| G: -5311.25950 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.05471 HOMO: -6.73754 LUMO: -0.45443 factor:1 | 1 (-1.42952) | -1 | -1 |
| G: -5311.25950 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.27061 HOMO: -6.24501 LUMO: 0.38096 factor:1 | 1 (-1.64542) | -1 | -1 |
| G: -5311.25950 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.14631 HOMO: -6.86815 LUMO: -0.91974 factor:1 | 1 (-1.52112) | -1 | -1 |
| G: -5311.25950 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.00557 HOMO: -7.40150 LUMO: 0.36191 factor:1 | 1 (-1.38038) | 1 | 1 |
| G: -5311.25950 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.11578 HOMO: -6.44094 LUMO: -0.64219 factor:1 | 1 (-1.49059) | -1 | -1 |
| G: -5311.25950 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.31690 HOMO: -6.69944 LUMO: -0.80001 factor:1 | 1 (-1.69170) | -1 | -1 |
| G: -5311.25950 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.00252 HOMO: -6.61509 LUMO: -0.70750 factor:1 | 1 (-1.37733) | -1 | -1 |
| G: -5311.25950 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.12522 HOMO: -7.52123 LUMO: 0.06803 factor:1 | 1 (-1.50003) | 1 | 1 |
| G: -5311.25950 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.01020 HOMO: -7.34163 LUMO: 0.30477 factor:1 | 1 (-1.38501) | 1 | 1 |
| G: -5311.25950 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.08067 HOMO: -6.68584 LUMO: -0.78641 factor:1 | 1 (-1.45548) | -1 | -1 |
| G: -5311.25950 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.06127 HOMO: -6.53890 LUMO: -0.50885 factor:1 | 1 (-1.43608) | -1 | -1 |
| G: -5311.25950 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.15706 HOMO: -6.75659 LUMO: -0.68845 factor:1 | 1 (-1.53186) | -1 | -1 |
| G: -5311.25950 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.65244 HOMO: -7.08857 LUMO: 0.43266 factor:1 | 1 (-2.02725) | 1 | 1 |
| G: -5311.25950 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.76240 HOMO: -6.28583 LUMO: -0.46804 factor:1 | 1 (-2.13721) | -1 | -1 |
| G: -5311.25950 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.95296 HOMO: -6.50080 LUMO: -0.24762 factor:1 | 1 (-2.32777) | -1 | -1 |
| G: -5311.25950 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.53309 HOMO: -6.45454 LUMO: -0.58504 factor:1 | 1 (-1.90790) | -1 | -1 |
| G: -5311.25950 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.78809 HOMO: -7.20558 LUMO: 0.20953 factor:1 | 1 (-2.16290) | 1 | 1 |
| G: -5311.25950 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.64134 HOMO: -6.35930 LUMO: -0.20681 factor:1 | 1 (-2.01615) | -1 | -1 |
| G: -5311.25950 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11578.02616 HOMO: -6.36202 LUMO: -0.14422 factor:1 | 1 (-2.40097) | -1 | -1 |
| G: -5311.25950 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.81554 HOMO: -6.20692 LUMO: 1.97827 factor:1 | 1 (-2.19035) | -1 | -1 |
| G: -5311.25950 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.89647 HOMO: -6.48719 LUMO: 1.74153 factor:1 | 1 (-2.27128) | -1 | -1 |
| G: -5311.25950 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.96118 HOMO: -6.84638 LUMO: 1.88575 factor:1 | 1 (-2.33599) | -1 | -1 |
| G: -5311.25950 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.97621 HOMO: -5.90759 LUMO: 2.00820 factor:1 | 1 (-1.35102) | -1 | -1 |
| G: -5311.25950 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.02353 HOMO: -6.56339 LUMO: 1.99732 factor:1 | 1 (-1.39834) | -1 | -1 |
| G: -5311.25950 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.14419 HOMO: -6.20692 LUMO: 1.75241 factor:1 | 1 (-1.51899) | -1 | -1 |
| G: -5311.25950 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.08429 HOMO: -6.16882 LUMO: 1.94017 factor:1 | 1 (-1.45910) | -1 | -1 |
| G: -5311.25950 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.99433 HOMO: -6.80829 LUMO: 1.78507 factor:1 | 1 (-1.36914) | -1 | -1 |
| G: -5311.25950 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.78886 HOMO: -6.58243 LUMO: 1.78235 factor:1 | 1 (-1.16367) | -1 | -1 |
| G: -5311.25950 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.83689 HOMO: -5.85045 LUMO: 1.82316 factor:1 | 1 (-1.21170) | -1 | -1 |
| G: -5311.25950 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.91945 HOMO: -5.93752 LUMO: 1.56465 factor:1 | 1 (-1.29426) | -1 | -1 |
| G: -5311.25950 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.97485 HOMO: -6.59604 LUMO: -0.53334 factor:1 | 1 (-1.34966) | -1 | -1 |
| G: -5311.25950 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.14516 HOMO: -7.06135 LUMO: 0.29660 factor:1 | 1 (-1.51997) | 1 | 1 |
| G: -5311.25950 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.85101 HOMO: -6.50352 LUMO: 1.61908 factor:1 | 1 (-1.22582) | -1 | -1 |
| G: -5311.25950 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.75041 HOMO: -6.68040 LUMO: -0.60681 factor:1 | 1 (-1.12522) | -1 | -1 |
| G: -5311.25950 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.88045 HOMO: -6.93618 LUMO: -1.09662 factor:1 | 1 (-1.25526) | -1 | -1 |
| G: -5311.25950 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.78189 HOMO: -6.72121 LUMO: -1.14016 factor:1 | 1 (-1.15670) | -1 | -1 |
| G: -5311.25950 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.06329 HOMO: -7.12394 LUMO: -1.24900 factor:1 | 1 (-1.43809) | -1 | -1 |
| G: -5311.25950 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.90037 HOMO: -6.71305 LUMO: -0.71566 factor:1 | 1 (-1.27518) | -1 | -1 |
| G: -5311.25950 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.05787 HOMO: -7.09401 LUMO: -0.86532 factor:1 | 1 (-1.43268) | -1 | -1 |
| G: -5311.25950 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11578.95440 HOMO: -7.08584 LUMO: -0.92519 factor:1 | 1 (-3.32920) | -1 | -1 |
| G: -5311.25950 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11578.00401 HOMO: -7.05591 LUMO: 0.11973 factor:1 | 1 (-2.37882) | -1 | -1 |
| G: -5311.25950 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11578.22633 HOMO: -7.14843 LUMO: -1.58370 factor:1 | 1 (-2.60114) | -1 | -1 |
| G: -5311.25950 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11578.35074 HOMO: -7.36884 LUMO: -1.97010 factor:1 | 1 (-2.72555) | -1 | -1 |
| G: -5311.25950 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.72037 HOMO: -6.81373 LUMO: -1.72248 factor:1 | 1 (-1.09518) | -1 | -1 |
| G: -5311.25950 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.85237 HOMO: -6.87360 LUMO: -1.03947 factor:1 | 1 (-1.22718) | -1 | -1 |
| G: -5311.25950 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.97158 HOMO: -7.02870 LUMO: -0.87349 factor:1 | 1 (-1.34639) | -1 | -1 |
| G: -5311.25950 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.81248 HOMO: -7.16476 LUMO: -1.18097 factor:1 | 1 (-1.18729) | -1 | -1 |
| G: -5311.25950 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.69759 HOMO: -7.51851 LUMO: 0.07891 factor:1 | 1 (-1.07240) | 1 | 1 |
| G: -5311.25950 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11578.44543 HOMO: -7.04231 LUMO: -0.83539 factor:1 | 1 (-2.82024) | -1 | -1 |
| G: -5311.25950 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.65519 HOMO: -6.83278 LUMO: -0.60137 factor:1 | 1 (-2.03000) | -1 | -1 |
| G: -5311.25950 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.75337 HOMO: -6.89809 LUMO: -1.19186 factor:1 | 1 (-2.12818) | -1 | -1 |
| G: -5311.25950 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.83933 HOMO: -7.16476 LUMO: -0.79185 factor:1 | 1 (-2.21414) | -1 | -1 |
| G: -5311.25950 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.96779 HOMO: -6.97156 LUMO: -1.25444 factor:1 | 1 (-2.34260) | -1 | -1 |
| G: -5311.25950 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.95855 HOMO: -6.84366 LUMO: -0.88437 factor:1 | 1 (-1.33336) | -1 | -1 |
| G: -5311.25950 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.21649 HOMO: -6.91986 LUMO: -1.12655 factor:1 | 1 (-1.59129) | -1 | -1 |
| G: -5311.25950 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.91822 HOMO: -6.49536 LUMO: -0.29660 factor:1 | 1 (-1.29303) | -1 | -1 |
| G: -5311.25950 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.98994 HOMO: -6.74842 LUMO: 0.42450 factor:1 | 1 (-2.36475) | -1 | -1 |
| G: -5311.25950 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.99277 HOMO: -7.34435 LUMO: 0.32109 factor:1 | 1 (-2.36758) | 1 | 1 |
| G: -5311.25950 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.87527 HOMO: -7.16476 LUMO: 0.28572 factor:1 | 1 (-2.25008) | 1 | 1 |
| G: -5311.25950 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.86178 HOMO: -6.74298 LUMO: -0.43538 factor:1 | 1 (-2.23659) | -1 | -1 |
| G: -5311.25950 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.93106 HOMO: -7.19469 LUMO: -1.61091 factor:1 | 1 (-2.30587) | -1 | -1 |
| G: -5311.25950 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11578.52731 HOMO: -7.35252 LUMO: -1.78235 factor:1 | 1 (-2.90212) | -1 | -1 |
| G: -5311.25950 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.20008 HOMO: -7.25456 LUMO: -1.66806 factor:1 | 1 (-1.57489) | -1 | -1 |
| G: -5311.25950 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11578.21245 HOMO: -7.54844 LUMO: -1.07213 factor:1 | 1 (-2.58726) | -1 | -1 |
| G: -5311.25950 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11578.08701 HOMO: -7.21918 LUMO: -1.55377 factor:1 | 1 (-2.46181) | -1 | -1 |
| G: -5311.25950 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.99424 HOMO: -7.01782 LUMO: -1.60547 factor:1 | 1 (-2.36905) | -1 | -1 |
| G: -5311.25950 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.67342 HOMO: -7.21646 LUMO: -1.53472 factor:1 | 1 (-2.04823) | -1 | -1 |
| G: -5311.25950 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.91821 HOMO: -6.73754 LUMO: -1.37417 factor:1 | 1 (-2.29302) | -1 | -1 |
| G: -5311.25950 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11578.06709 HOMO: -6.78924 LUMO: 0.66396 factor:1 | 1 (-2.44190) | -1 | -1 |
| G: -5311.25950 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.82091 HOMO: -6.82734 LUMO: 0.61226 factor:1 | 1 (-2.19571) | -1 | -1 |
| G: -5311.25950 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.66515 HOMO: -6.74026 LUMO: 0.65579 factor:1 | 1 (-2.03996) | -1 | -1 |
| G: -5311.25950 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.37486 HOMO: -7.10489 LUMO: -1.30887 factor:1 | 1 (-1.74966) | -1 | -1 |
| G: -5311.25950 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.47339 HOMO: -7.05047 LUMO: 0.42722 factor:1 | 1 (-1.84820) | -1 | -1 |
| G: -5311.25950 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.45910 HOMO: -6.61237 LUMO: 1.30887 factor:1 | 1 (-1.83391) | -1 | -1 |
| G: -5311.25950 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.26756 HOMO: -7.05863 LUMO: 0.59049 factor:1 | 1 (-1.64237) | -1 | -1 |
| G: -5311.25950 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.88371 HOMO: -6.26406 LUMO: 0.78641 factor:1 | 1 (-2.25852) | -1 | -1 |
| G: -5311.25950 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.62332 HOMO: -6.70489 LUMO: 0.67756 factor:1 | 1 (-1.99813) | -1 | -1 |
| G: -5311.25950 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.62354 HOMO: -6.78652 LUMO: -0.94968 factor:1 | 1 (-1.99835) | -1 | -1 |
| G: -5311.25950 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.48607 HOMO: -6.36202 LUMO: -0.94424 factor:1 | 1 (-1.86088) | -1 | -1 |
| G: -5311.25950 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.54626 HOMO: -6.81645 LUMO: -1.09934 factor:1 | 1 (-1.92107) | -1 | -1 |
| G: -5311.25950 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.46640 HOMO: -7.07224 LUMO: 0.85988 factor:1 | 1 (-1.84120) | 1 | 1 |
| G: -5311.25950 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.40193 HOMO: -7.02326 LUMO: 1.10206 factor:1 | 1 (-1.77674) | -1 | -1 |
| G: -5311.25950 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.17673 HOMO: -6.71305 LUMO: 0.84627 factor:1 | 1 (-1.55154) | -1 | -1 |
| G: -5311.25950 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.32386 HOMO: -7.27360 LUMO: 0.88165 factor:1 | 1 (-1.69867) | 1 | 1 |
| G: -5311.25950 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.29080 HOMO: -6.84911 LUMO: 0.59865 factor:1 | 1 (-1.66561) | -1 | -1 |
| G: -5311.25950 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.73803 HOMO: -6.75114 LUMO: -2.49801 factor:1 | 1 (-1.11284) | -1 | -1 |
| G: -5311.25950 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.10696 HOMO: -6.97156 LUMO: 0.53606 factor:1 | 1 (-1.48177) | -1 | -1 |
| G: -5311.25950 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.27080 HOMO: -6.54434 LUMO: 0.73199 factor:1 | 1 (-1.64561) | -1 | -1 |
| G: -5311.25950 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.31456 HOMO: -6.21236 LUMO: 0.99866 factor:1 | 1 (-1.68936) | -1 | -1 |
| G: -5311.25950 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.44906 HOMO: -6.34025 LUMO: 0.50341 factor:1 | 1 (-1.82387) | -1 | -1 |
| G: -5311.25950 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.46435 HOMO: -6.59876 LUMO: -0.69389 factor:1 | 1 (-1.83916) | -1 | -1 |
| G: -5311.25950 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.85116 HOMO: -6.54978 LUMO: -1.00682 factor:1 | 1 (-2.22597) | -1 | -1 |
| G: -5311.25950 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11578.06088 HOMO: -6.82462 LUMO: -0.98777 factor:1 | 1 (-2.43569) | -1 | -1 |
| G: -5311.25950 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11578.02202 HOMO: -6.85455 LUMO: -0.68573 factor:1 | 1 (-2.39683) | -1 | -1 |
| G: -5311.25950 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11578.21381 HOMO: -7.55388 LUMO: -0.03265 factor:1 | 1 (-2.58862) | 1 | 1 |
| G: -5311.25950 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.77380 HOMO: -6.77019 LUMO: -0.71838 factor:1 | 1 (-2.14861) | -1 | -1 |
| G: -5311.25950 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11578.00850 HOMO: -6.84911 LUMO: -1.25444 factor:1 | 1 (-2.38331) | -1 | -1 |
| G: -5311.25950 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.95089 HOMO: -6.95251 LUMO: -1.03675 factor:1 | 1 (-2.32570) | -1 | -1 |
| G: -5311.25950 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11578.06075 HOMO: -6.80829 LUMO: -0.77280 factor:1 | 1 (-2.43556) | -1 | -1 |
| G: -5311.25950 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.89399 HOMO: -6.94162 LUMO: -0.94151 factor:1 | 1 (-2.26880) | -1 | -1 |
| G: -5311.25950 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11578.14146 HOMO: -6.89809 LUMO: -0.90886 factor:1 | 1 (-2.51626) | -1 | -1 |
| G: -5311.25950 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.70452 HOMO: -6.85183 LUMO: -0.88981 factor:1 | 1 (-2.07933) | -1 | -1 |
| G: -5311.25950 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.86997 HOMO: -6.51985 LUMO: -0.84627 factor:1 | 1 (-2.24478) | -1 | -1 |
| G: -5311.25950 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.77571 HOMO: -6.83278 LUMO: -1.08029 factor:1 | 1 (-2.15052) | -1 | -1 |
| G: -5311.25950 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.81361 HOMO: -6.91986 LUMO: 0.66396 factor:1 | 1 (-2.18842) | -1 | -1 |
| G: -5311.25950 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.86338 HOMO: -6.94162 LUMO: 0.50885 factor:1 | 1 (-2.23819) | -1 | -1 |
| G: -5311.25950 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11578.22701 HOMO: -6.94435 LUMO: 0.80546 factor:1 | 1 (-2.60182) | -1 | -1 |
| G: -5311.25950 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11578.04143 HOMO: -6.74298 LUMO: -0.81634 factor:1 | 1 (-2.41624) | -1 | -1 |
| G: -5311.25950 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11578.00494 HOMO: -7.04503 LUMO: 1.15921 factor:1 | 1 (-2.37974) | -1 | -1 |
| G: -5311.25950 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.23273 HOMO: -6.76475 LUMO: 0.75920 factor:1 | 1 (-1.60754) | -1 | -1 |
| G: -5311.25950 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.31940 HOMO: -7.05047 LUMO: 0.68845 factor:1 | 1 (-1.69421) | -1 | -1 |
| G: -5311.25950 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.90151 HOMO: -7.12666 LUMO: 0.60681 factor:1 | 1 (-1.27632) | 1 | 1 |
| G: -5311.25950 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.00786 HOMO: -6.90897 LUMO: -1.22723 factor:1 | 1 (-1.38266) | -1 | -1 |
| G: -5311.25950 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.24511 HOMO: -7.10761 LUMO: 0.58232 factor:1 | 1 (-1.61992) | 1 | 1 |
| G: -5311.25950 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.43682 HOMO: -6.57427 LUMO: 0.71294 factor:1 | 1 (-1.81163) | -1 | -1 |
| G: -5311.25950 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.83966 HOMO: -6.22597 LUMO: 0.99322 factor:1 | 1 (-1.21447) | -1 | -1 |
| G: -5311.25950 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.07820 HOMO: -6.83550 LUMO: -0.77825 factor:1 | 1 (-1.45301) | -1 | -1 |
| G: -5311.25950 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.27589 HOMO: -7.14843 LUMO: 0.44627 factor:1 | 1 (-1.65070) | 1 | 1 |
| G: -5311.25950 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.84099 HOMO: -7.08040 LUMO: 0.78913 factor:1 | 1 (-2.21580) | 1 | 1 |
| G: -5311.25950 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.84602 HOMO: -6.81373 LUMO: -0.93879 factor:1 | 1 (-2.22083) | -1 | -1 |
| G: -5311.25950 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.77715 HOMO: -6.95251 LUMO: 0.22585 factor:1 | 1 (-2.15196) | -1 | -1 |
| G: -5311.25950 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.77601 HOMO: -7.13483 LUMO: -1.25444 factor:1 | 1 (-2.15082) | -1 | -1 |
| G: -5311.25950 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.84099 HOMO: -6.37835 LUMO: -1.54289 factor:1 | 1 (-2.21580) | -1 | -1 |
| G: -5311.25950 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.76071 HOMO: -6.53617 LUMO: -1.43948 factor:1 | 1 (-2.13552) | -1 | -1 |
| G: -5311.25950 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.82929 HOMO: -6.38379 LUMO: 0.16055 factor:1 | 1 (-2.20410) | -1 | -1 |
| G: -5311.25950 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.83998 HOMO: -6.53617 LUMO: 0.15783 factor:1 | 1 (-2.21479) | -1 | -1 |
| G: -5311.25950 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11578.06382 HOMO: -6.79740 LUMO: -0.17960 factor:1 | 1 (-2.43863) | -1 | -1 |
| G: -5311.25950 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11578.05656 HOMO: -6.26678 LUMO: -0.41361 factor:1 | 1 (-2.43136) | -1 | -1 |
| G: -5311.25950 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.78877 HOMO: -6.35658 LUMO: -0.24218 factor:1 | 1 (-2.16358) | -1 | -1 |
| G: -5311.25950 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.94172 HOMO: -6.48175 LUMO: -0.71566 factor:1 | 1 (-2.31653) | -1 | -1 |
| G: -5311.25950 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.96847 HOMO: -6.21508 LUMO: -0.40001 factor:1 | 1 (-2.34328) | -1 | -1 |
| G: -5311.25950 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.95070 HOMO: -6.51985 LUMO: -0.32654 factor:1 | 1 (-2.32551) | -1 | -1 |
| G: -5311.25950 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.86142 HOMO: -6.45182 LUMO: -0.66396 factor:1 | 1 (-2.23623) | -1 | -1 |
| G: -5311.25950 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.97636 HOMO: -6.51441 LUMO: -0.65307 factor:1 | 1 (-2.35117) | -1 | -1 |
| G: -5311.25950 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: -0.92519 factor:1 | 1 (-2.09054) | -1 | -1 |
| G: -5311.25950 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11578.05544 HOMO: -6.67223 LUMO: -0.58232 factor:1 | 1 (-2.43025) | -1 | -1 |
| G: -5311.25950 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11578.06317 HOMO: -6.10351 LUMO: -0.45987 factor:1 | 1 (-2.43798) | -1 | -1 |
| G: -5311.25950 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11578.09218 HOMO: -6.13889 LUMO: -0.50341 factor:1 | 1 (-2.46698) | -1 | -1 |
| G: -5311.25950 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.77130 HOMO: -6.63141 LUMO: -0.28300 factor:1 | 1 (-2.14611) | -1 | -1 |
| G: -5311.25950 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.76115 HOMO: -6.37563 LUMO: -0.22858 factor:1 | 1 (-2.13596) | -1 | -1 |
| G: -5311.25950 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11578.03054 HOMO: -6.37019 LUMO: 0.11429 factor:1 | 1 (-2.40535) | -1 | -1 |
| G: -5311.25950 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.76855 HOMO: -6.23957 LUMO: 0.28844 factor:1 | 1 (-2.14336) | -1 | -1 |
| G: -5311.25950 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.89979 HOMO: -6.41372 LUMO: -0.53879 factor:1 | 1 (-2.27460) | -1 | -1 |
| G: -5311.25950 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.75244 HOMO: -7.06680 LUMO: 0.32654 factor:1 | 1 (-2.12725) | 1 | 1 |
| G: -5311.25950 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.68357 HOMO: -6.50896 LUMO: -0.73743 factor:1 | 1 (-2.05838) | -1 | -1 |
| G: -5311.25950 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.96059 HOMO: -6.42189 LUMO: -0.28572 factor:1 | 1 (-1.33540) | -1 | -1 |
| G: -5311.25950 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.28223 HOMO: -6.79740 LUMO: -0.25851 factor:1 | 1 (-1.65704) | -1 | -1 |
| G: -5311.25950 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.07545 HOMO: -6.32393 LUMO: 0.17960 factor:1 | 1 (-1.45026) | -1 | -1 |
| G: -5311.25950 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.03052 HOMO: -6.65046 LUMO: 0.03537 factor:1 | 1 (-1.40533) | -1 | -1 |
| G: -5311.25950 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.86180 HOMO: -6.60148 LUMO: 0.07619 factor:1 | 1 (-2.23661) | -1 | -1 |
| G: -5311.25950 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.72137 HOMO: -6.57971 LUMO: 0.11429 factor:1 | 1 (-2.09617) | -1 | -1 |
| G: -5311.25950 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11578.10442 HOMO: -6.88448 LUMO: -1.21907 factor:1 | 1 (-2.47923) | -1 | -1 |
| G: -5311.25950 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.94834 HOMO: -6.97700 LUMO: 0.36463 factor:1 | 1 (-2.32314) | -1 | -1 |
| G: -5311.25950 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.93908 HOMO: -6.73210 LUMO: -0.84083 factor:1 | 1 (-2.31389) | -1 | -1 |
| G: -5311.25950 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11578.05239 HOMO: -6.21236 LUMO: -0.68845 factor:1 | 1 (-2.42720) | -1 | -1 |
| G: -5311.25950 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.78537 HOMO: -6.35658 LUMO: -0.82995 factor:1 | 1 (-2.16018) | -1 | -1 |
| G: -5311.25950 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.85157 HOMO: -6.75114 LUMO: -0.94424 factor:1 | 1 (-2.22638) | -1 | -1 |
| G: -5311.25950 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11578.03854 HOMO: -6.74026 LUMO: -1.46125 factor:1 | 1 (-2.41335) | -1 | -1 |
| G: -5311.25950 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11578.06763 HOMO: -7.06952 LUMO: 0.91974 factor:1 | 1 (-2.44244) | 1 | 1 |
| G: -5311.25950 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11578.09294 HOMO: -7.08857 LUMO: 0.74559 factor:1 | 1 (-2.46775) | 1 | 1 |
| G: -5311.25950 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.93631 HOMO: -6.74298 LUMO: 1.03131 factor:1 | 1 (-2.31112) | -1 | -1 |
| G: -5311.25950 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.77212 HOMO: -6.74842 LUMO: -1.77962 factor:1 | 1 (-2.14692) | -1 | -1 |
| G: -5311.25950 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.61630 HOMO: -6.82462 LUMO: -1.61908 factor:1 | 1 (-1.99111) | -1 | -1 |
| G: -5311.25950 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.80455 HOMO: -7.17020 LUMO: -1.02043 factor:1 | 1 (-2.17936) | -1 | -1 |
| G: -5311.25950 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.87865 HOMO: -6.26406 LUMO: -0.96328 factor:1 | 1 (-2.25346) | -1 | -1 |
| G: -5311.25950 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.74014 HOMO: -6.50896 LUMO: -0.38640 factor:1 | 1 (-2.11495) | -1 | -1 |
| G: -5311.25950 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.56972 HOMO: -7.27632 LUMO: -1.17553 factor:1 | 1 (-1.94453) | -1 | -1 |
| G: -5311.25950 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.44552 HOMO: -6.54162 LUMO: -1.36873 factor:1 | 1 (-1.82033) | -1 | -1 |
| G: -5311.25950 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.59935 HOMO: -6.42733 LUMO: -1.15648 factor:1 | 1 (-1.97416) | -1 | -1 |
| G: -5311.25950 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.52329 HOMO: -6.73754 LUMO: -2.58780 factor:1 | 1 (-1.89810) | -1 | -1 |
| G: -5311.25950 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.71383 HOMO: -7.20285 LUMO: 0.75103 factor:1 | 1 (-2.08864) | 1 | 1 |
| G: -5311.25950 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.42596 HOMO: -6.98788 LUMO: 0.34831 factor:1 | 1 (-1.80077) | -1 | -1 |
| G: -5311.25950 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.65685 HOMO: -6.80013 LUMO: -1.11567 factor:1 | 1 (-2.03166) | -1 | -1 |
| G: -5311.25950 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.50610 HOMO: -6.67767 LUMO: -0.82450 factor:1 | 1 (-1.88091) | -1 | -1 |
| G: -5311.25950 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.60893 HOMO: -6.84911 LUMO: -0.21497 factor:1 | 1 (-1.98374) | -1 | -1 |
| G: -5311.25950 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.82452 HOMO: -6.23141 LUMO: 0.21769 factor:1 | 1 (-2.19933) | -1 | -1 |
| G: -5311.25950 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.53584 HOMO: -6.68312 LUMO: 0.16327 factor:1 | 1 (-1.91065) | -1 | -1 |
| G: -5311.25950 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.48803 HOMO: -7.04503 LUMO: -1.04220 factor:1 | 1 (-1.86284) | -1 | -1 |
| G: -5311.25950 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.43894 HOMO: -6.67495 LUMO: -0.71294 factor:1 | 1 (-1.81375) | -1 | -1 |
| G: -5311.25950 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.72343 HOMO: -6.70216 LUMO: -0.55239 factor:1 | 1 (-2.09824) | -1 | -1 |
| G: -5311.25950 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.63081 HOMO: -6.60420 LUMO: -0.71294 factor:1 | 1 (-2.00562) | -1 | -1 |
| G: -5311.25950 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.70928 HOMO: -7.40694 LUMO: 0.11973 factor:1 | 1 (-2.08409) | 1 | 1 |
| G: -5311.25950 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.74349 HOMO: -6.58788 LUMO: -0.29116 factor:1 | 1 (-2.11830) | -1 | -1 |
| G: -5311.25950 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.83481 HOMO: -6.63686 LUMO: -0.32654 factor:1 | 1 (-2.20962) | -1 | -1 |
| G: -5311.25950 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11578.05411 HOMO: -6.85183 LUMO: -0.95512 factor:1 | 1 (-2.42892) | -1 | -1 |
| G: -5311.25950 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.79761 HOMO: -6.82189 LUMO: -0.88165 factor:1 | 1 (-2.17242) | -1 | -1 |
| G: -5311.25950 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.76428 HOMO: -6.97428 LUMO: -1.03947 factor:1 | 1 (-2.13909) | -1 | -1 |
| G: -5311.25950 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.75108 HOMO: -6.51441 LUMO: -0.05714 factor:1 | 1 (-2.12589) | -1 | -1 |
| G: -5311.25950 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.91136 HOMO: -6.61509 LUMO: -0.77008 factor:1 | 1 (-2.28616) | -1 | -1 |
| G: -5311.25950 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.70488 HOMO: -7.36340 LUMO: 0.29116 factor:1 | 1 (-2.07968) | 1 | 1 |
| G: -5311.25950 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.78934 HOMO: -6.64230 LUMO: -0.79185 factor:1 | 1 (-2.16415) | -1 | -1 |
| G: -5311.25950 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.48343 HOMO: -6.56883 LUMO: -1.03403 factor:1 | 1 (-1.85824) | -1 | -1 |
| G: -5311.25950 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.43818 HOMO: -6.69400 LUMO: -0.77825 factor:1 | 1 (-1.81299) | -1 | -1 |
| G: -5311.25950 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.54229 HOMO: -6.37019 LUMO: -0.79185 factor:1 | 1 (-1.91710) | -1 | -1 |
| G: -5311.25950 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.43543 HOMO: -6.49808 LUMO: -0.94424 factor:1 | 1 (-1.81024) | -1 | -1 |
| G: -5311.25950 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.34990 HOMO: -6.91713 LUMO: -0.75376 factor:1 | 1 (-1.72471) | -1 | -1 |
| G: -5311.25950 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.39061 HOMO: -7.13755 LUMO: 0.41361 factor:1 | 1 (-1.76542) | 1 | 1 |
| G: -5311.25950 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.64136 HOMO: -7.12122 LUMO: 0.39457 factor:1 | 1 (-2.01617) | 1 | 1 |
| G: -5311.25950 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.42732 HOMO: -6.59332 LUMO: -0.57144 factor:1 | 1 (-1.80213) | -1 | -1 |
| G: -5311.25950 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.73405 HOMO: -6.62325 LUMO: -0.66940 factor:1 | 1 (-2.10886) | -1 | -1 |
| G: -5311.25950 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.48950 HOMO: -6.90897 LUMO: -0.08708 factor:1 | 1 (-1.86431) | -1 | -1 |
| G: -5311.25950 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.33015 HOMO: -6.65591 LUMO: -0.81090 factor:1 | 1 (-1.70496) | -1 | -1 |
| G: -5311.25950 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.27763 HOMO: -6.65318 LUMO: -0.94696 factor:1 | 1 (-1.65244) | -1 | -1 |
| G: -5311.25950 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.17774 HOMO: -6.96067 LUMO: -1.03675 factor:1 | 1 (-1.55255) | -1 | -1 |
| G: -5311.25950 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.93550 HOMO: -6.23141 LUMO: -0.66396 factor:1 | 1 (-1.31031) | -1 | -1 |
| G: -5311.25950 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.42231 HOMO: -6.52529 LUMO: -0.78369 factor:1 | 1 (-1.79712) | -1 | -1 |
| G: -5311.25950 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.22381 HOMO: -6.39468 LUMO: -0.40817 factor:1 | 1 (-1.59861) | -1 | -1 |
| G: -5311.25950 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.11708 HOMO: -6.76203 LUMO: -0.20409 factor:1 | 1 (-1.49189) | -1 | -1 |
| G: -5311.25950 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.60969 HOMO: -6.96611 LUMO: -0.90342 factor:1 | 1 (-1.98450) | -1 | -1 |
| G: -5311.25950 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.16239 HOMO: -6.54706 LUMO: -0.87893 factor:1 | 1 (-1.53720) | -1 | -1 |
| G: -5311.25950 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.27962 HOMO: -7.24367 LUMO: -0.97689 factor:1 | 1 (-1.65443) | -1 | -1 |
| G: -5311.25950 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.36359 HOMO: -6.61781 LUMO: 1.43404 factor:1 | 1 (-1.73840) | -1 | -1 |
| G: -5311.25950 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11578.11743 HOMO: -6.17971 LUMO: 1.79867 factor:1 | 1 (-2.49224) | -1 | -1 |
| G: -5311.25950 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11578.01816 HOMO: -5.73344 LUMO: 2.13609 factor:1 | 1 (-2.39297) | -1 | -1 |
| G: -5311.25950 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11578.34641 HOMO: -6.72121 LUMO: 2.06807 factor:1 | 1 (-2.72122) | -1 | -1 |
| G: -5311.25950 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.81614 HOMO: -6.91169 LUMO: 2.02997 factor:1 | 1 (-2.19095) | -1 | -1 |
| G: -5311.25950 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11578.72579 HOMO: -7.06408 LUMO: 1.41499 factor:1 | 1 (-3.10060) | 1 | 1 |
| G: -5311.25950 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11578.20976 HOMO: -6.94162 LUMO: -0.90070 factor:1 | 1 (-2.58456) | -1 | -1 |
| G: -5311.25950 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11578.40336 HOMO: -7.09401 LUMO: 0.35103 factor:1 | 1 (-2.77817) | 1 | 1 |
| G: -5311.25950 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11578.39887 HOMO: -6.78652 LUMO: 0.91974 factor:1 | 1 (-2.77368) | -1 | -1 |
| G: -5311.25950 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11578.77831 HOMO: -6.32937 LUMO: -1.89119 factor:1 | 1 (-3.15312) | -1 | -1 |
| G: -5311.25950 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11578.21773 HOMO: -7.12666 LUMO: -1.06397 factor:1 | 1 (-2.59254) | -1 | -1 |
| G: -5311.25950 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11578.53074 HOMO: -6.38107 LUMO: -1.43132 factor:1 | 1 (-2.90555) | -1 | -1 |
| G: -5311.25950 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11579.08836 HOMO: -7.09129 LUMO: 0.08980 factor:1 | 1 (-3.46317) | 1 | 1 |
| G: -5311.25950 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11578.82120 HOMO: -6.31304 LUMO: -0.57960 factor:1 | 1 (-3.19600) | -1 | -1 |
| G: -5311.25950 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11578.27542 HOMO: -6.94435 LUMO: -0.74287 factor:1 | 1 (-2.65023) | -1 | -1 |
| G: -5311.25950 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11578.38184 HOMO: -6.35658 LUMO: -1.53472 factor:1 | 1 (-2.75665) | -1 | -1 |
| G: -5311.25950 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11578.16682 HOMO: -6.39740 LUMO: -1.48846 factor:1 | 1 (-2.54163) | -1 | -1 |
| G: -5311.25950 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11579.02120 HOMO: -7.05319 LUMO: -0.33198 factor:1 | 1 (-3.39601) | -1 | -1 |
| G: -5311.25950 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11578.83913 HOMO: -6.68040 LUMO: -0.09252 factor:1 | 1 (-3.21394) | -1 | -1 |
| G: -5311.25950 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11578.03351 HOMO: -6.35930 LUMO: -0.43266 factor:1 | 1 (-2.40832) | -1 | -1 |
| G: -5311.25950 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11578.23299 HOMO: -6.59604 LUMO: -1.45853 factor:1 | 1 (-2.60780) | -1 | -1 |
| G: -5311.25950 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.84477 HOMO: -6.46270 LUMO: -1.49391 factor:1 | 1 (-2.21958) | -1 | -1 |
| G: -5311.25950 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.79947 HOMO: -7.05863 LUMO: -1.04764 factor:1 | 1 (-1.17428) | -1 | -1 |
| G: -5311.25950 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.84769 HOMO: -7.14027 LUMO: -0.81634 factor:1 | 1 (-1.22250) | -1 | -1 |
| G: -5311.25950 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.86249 HOMO: -6.80285 LUMO: -0.74287 factor:1 | 1 (-1.23730) | -1 | -1 |
| G: -5311.25950 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.62652 HOMO: -6.53890 LUMO: -1.13471 factor:1 | 1 (-1.00132) | -1 | -1 |
| G: -5311.25950 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.73604 HOMO: -6.49808 LUMO: -1.35513 factor:1 | 1 (-1.11085) | -1 | -1 |
| G: -5311.25950 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.66398 HOMO: -6.75931 LUMO: -1.49663 factor:1 | 1 (-2.03879) | -1 | -1 |
| G: -5311.25950 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.89965 HOMO: -6.84638 LUMO: -0.77552 factor:1 | 1 (-2.27446) | -1 | -1 |
| G: -5311.25950 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.91835 HOMO: -6.65863 LUMO: -1.34696 factor:1 | 1 (-2.29316) | -1 | -1 |
| G: -5311.25950 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.59715 HOMO: -6.25590 LUMO: -2.36467 factor:1 | 1 (-1.97195) | -1 | -1 |
| G: -5311.25950 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.86385 HOMO: -7.24911 LUMO: 0.33470 factor:1 | 1 (-1.23866) | 1 | 1 |
| G: -5311.25950 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.86021 HOMO: -6.65863 LUMO: -0.75648 factor:1 | 1 (-1.23502) | -1 | -1 |
| G: -5311.25950 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.02035 HOMO: -6.31576 LUMO: -0.83267 factor:1 | 1 (-1.39515) | -1 | -1 |
| G: -5311.25950 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.22378 HOMO: -6.64774 LUMO: -0.66124 factor:1 | 1 (-1.59859) | -1 | -1 |
| G: -5311.25950 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.09305 HOMO: -6.75387 LUMO: -1.00138 factor:1 | 1 (-1.46786) | -1 | -1 |
| G: -5311.25950 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.71770 HOMO: -6.52529 LUMO: -0.68301 factor:1 | 1 (-1.09251) | -1 | -1 |
| G: -5311.25950 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.80674 HOMO: -6.59332 LUMO: -0.68028 factor:1 | 1 (-1.18155) | -1 | -1 |
| G: -5311.25950 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.72845 HOMO: -5.98650 LUMO: 0.31565 factor:1 | 1 (-1.10326) | -1 | -1 |
| G: -5311.25950 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.05586 HOMO: -6.59876 LUMO: 0.22585 factor:1 | 1 (-1.43067) | -1 | -1 |
| G: -5311.25950 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.82402 HOMO: -6.72121 LUMO: 0.10340 factor:1 | 1 (-1.19882) | -1 | -1 |
| G: -5311.25950 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.98347 HOMO: -6.09807 LUMO: 0.20136 factor:1 | 1 (-1.35828) | -1 | -1 |
| G: -5311.25950 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.21616 HOMO: -6.31576 LUMO: 0.06259 factor:1 | 1 (-1.59097) | -1 | -1 |
| G: -5311.25950 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.55585 HOMO: -6.35658 LUMO: -0.58232 factor:1 | 1 (-0.93066) | -1 | -1 |
| G: -5311.25950 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.69454 HOMO: -6.34842 LUMO: -0.55783 factor:1 | 1 (-1.06935) | -1 | -1 |
| G: -5311.25950 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.89047 HOMO: -6.47359 LUMO: -0.57144 factor:1 | 1 (-1.26528) | -1 | -1 |
| G: -5311.25950 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.68799 HOMO: -6.42189 LUMO: -0.09796 factor:1 | 1 (-1.06280) | -1 | -1 |
| G: -5311.25950 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.13257 HOMO: -6.35658 LUMO: -0.31293 factor:1 | 1 (-1.50737) | -1 | -1 |
| G: -5311.25950 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.19061 HOMO: -7.35524 LUMO: 0.10340 factor:1 | 1 (-1.56542) | 1 | 1 |
| G: -5311.25950 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.92418 HOMO: -7.10217 LUMO: 0.36463 factor:1 | 1 (-1.29899) | 1 | 1 |
| G: -5311.25950 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.76323 HOMO: -6.43549 LUMO: -0.56872 factor:1 | 1 (-1.13803) | -1 | -1 |
| G: -5311.25950 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.61057 HOMO: -6.50080 LUMO: -0.71294 factor:1 | 1 (-0.98538) | -1 | -1 |
| G: -5311.25950 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11578.08398 HOMO: -6.59060 LUMO: -0.57960 factor:1 | 1 (-2.45879) | -1 | -1 |
| G: -5311.25950 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11579.01891 HOMO: -6.78924 LUMO: -0.31565 factor:1 | 1 (-3.39372) | -1 | -1 |
| G: -5311.25950 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11578.31131 HOMO: -6.35658 LUMO: 0.07891 factor:1 | 1 (-2.68612) | -1 | -1 |
| G: -5311.25950 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11578.02292 HOMO: -6.74026 LUMO: -0.87621 factor:1 | 1 (-2.39773) | -1 | -1 |
| G: -5311.25950 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.78320 HOMO: -6.54434 LUMO: 0.81906 factor:1 | 1 (-1.15801) | -1 | -1 |
| G: -5311.25950 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.75087 HOMO: -6.66135 LUMO: 1.40955 factor:1 | 1 (-1.12568) | -1 | -1 |
| G: -5311.25950 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.07145 HOMO: -6.73754 LUMO: -2.54971 factor:1 | 1 (-1.44626) | -1 | -1 |
| G: -5311.25950 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.99123 HOMO: -6.65318 LUMO: 0.69389 factor:1 | 1 (-1.36604) | -1 | -1 |
| G: -5311.25950 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.66284 HOMO: -6.73482 LUMO: 0.62858 factor:1 | 1 (-1.03765) | -1 | -1 |
| G: -5311.25950 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.77301 HOMO: -6.83550 LUMO: 0.68573 factor:1 | 1 (-2.14782) | -1 | -1 |
| G: -5311.25950 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11578.40494 HOMO: -6.83278 LUMO: 0.45987 factor:1 | 1 (-2.77975) | -1 | -1 |
| G: -5311.25950 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.74382 HOMO: -6.78380 LUMO: 0.68301 factor:1 | 1 (-2.11862) | -1 | -1 |
| G: -5311.25950 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.99171 HOMO: -6.90625 LUMO: 1.36601 factor:1 | 1 (-2.36652) | -1 | -1 |
| G: -5311.25950 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.68654 HOMO: -6.82734 LUMO: 1.48302 factor:1 | 1 (-2.06134) | -1 | -1 |
| G: -5311.25950 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.69530 HOMO: -6.44094 LUMO: -0.94424 factor:1 | 1 (-2.07011) | -1 | -1 |
| G: -5311.25950 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.91348 HOMO: -6.91441 LUMO: 0.28844 factor:1 | 1 (-2.28829) | -1 | -1 |
| G: -5311.25950 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.92741 HOMO: -6.49808 LUMO: -0.51157 factor:1 | 1 (-2.30222) | -1 | -1 |
| G: -5311.25950 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.50670 HOMO: -7.09673 LUMO: -0.06259 factor:1 | 1 (-1.88150) | 1 | 1 |
| G: -5311.25950 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11578.06241 HOMO: -6.77019 LUMO: 0.92247 factor:1 | 1 (-2.43722) | -1 | -1 |
| G: -5311.25950 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.97402 HOMO: -6.75931 LUMO: 1.13744 factor:1 | 1 (-2.34883) | -1 | -1 |
| G: -5311.25950 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11578.26331 HOMO: -6.15794 LUMO: 1.12383 factor:1 | 1 (-2.63812) | -1 | -1 |
| G: -5311.25950 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.73931 HOMO: -6.59604 LUMO: 1.19458 factor:1 | 1 (-1.11412) | -1 | -1 |
| G: -5311.25950 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.83144 HOMO: -7.09401 LUMO: 0.60137 factor:1 | 1 (-1.20625) | 1 | 1 |
| G: -5311.25950 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.57781 HOMO: -6.34025 LUMO: 0.48164 factor:1 | 1 (-0.95262) | -1 | -1 |
| G: -5311.25950 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.89564 HOMO: -6.72665 LUMO: -2.47624 factor:1 | 1 (-1.27045) | -1 | -1 |
| G: -5311.25950 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.04369 HOMO: -6.48175 LUMO: 0.58232 factor:1 | 1 (-1.41850) | -1 | -1 |
| G: -5311.25950 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.61098 HOMO: -6.94162 LUMO: 0.28300 factor:1 | 1 (-0.98579) | -1 | -1 |
| G: -5311.25950 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11578.45460 HOMO: -6.65591 LUMO: 0.57144 factor:1 | 1 (-2.82941) | -1 | -1 |
| G: -5311.25950 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.63078 HOMO: -6.58788 LUMO: -1.03947 factor:1 | 1 (-2.00559) | -1 | -1 |
| G: -5311.25950 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.76730 HOMO: -7.18108 LUMO: 0.37824 factor:1 | 1 (-2.14211) | 1 | 1 |
| G: -5311.25950 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.91810 HOMO: -6.63958 LUMO: -1.52112 factor:1 | 1 (-2.29291) | -1 | -1 |
| G: -5311.25950 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11578.14880 HOMO: -6.12528 LUMO: -0.53606 factor:1 | 1 (-2.52361) | -1 | -1 |
| G: -5311.25950 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11578.33079 HOMO: -6.22324 LUMO: -0.87893 factor:1 | 1 (-2.70560) | -1 | -1 |
| G: -5311.25950 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11578.37721 HOMO: -6.62053 LUMO: -0.91974 factor:1 | 1 (-2.75202) | -1 | -1 |
| G: -5311.25950 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.91239 HOMO: -6.84366 LUMO: -0.83811 factor:1 | 1 (-2.28720) | -1 | -1 |
| G: -5311.25950 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.64634 HOMO: -7.26000 LUMO: 0.25851 factor:1 | 1 (-2.02115) | 1 | 1 |
| G: -5311.25950 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.88866 HOMO: -6.49536 LUMO: -0.63403 factor:1 | 1 (-2.26347) | -1 | -1 |
| G: -5311.25950 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.93949 HOMO: -6.45726 LUMO: -0.77825 factor:1 | 1 (-2.31430) | -1 | -1 |
| G: -5311.25950 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.66830 HOMO: -6.74570 LUMO: -0.75103 factor:1 | 1 (-2.04311) | -1 | -1 |
| G: -5311.25950 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11578.10924 HOMO: -7.20285 LUMO: 0.10612 factor:1 | 1 (-2.48405) | 1 | 1 |
| G: -5311.25950 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11578.33316 HOMO: -6.45182 LUMO: -0.56600 factor:1 | 1 (-2.70797) | -1 | -1 |
| G: -5311.25950 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11578.24845 HOMO: -6.83278 LUMO: -0.71838 factor:1 | 1 (-2.62326) | -1 | -1 |
| G: -5311.25950 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11578.01057 HOMO: -7.01510 LUMO: -1.09662 factor:1 | 1 (-2.38538) | -1 | -1 |
| G: -5311.25950 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.89724 HOMO: -6.48719 LUMO: 0.16871 factor:1 | 1 (-1.27205) | -1 | -1 |
| G: -5311.25950 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.74214 HOMO: -7.30898 LUMO: 0.26667 factor:1 | 1 (-1.11695) | 1 | 1 |
| G: -5311.25950 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.87251 HOMO: -6.68856 LUMO: -0.78641 factor:1 | 1 (-1.24732) | -1 | -1 |
| G: -5311.25950 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.94647 HOMO: -6.56883 LUMO: -1.00682 factor:1 | 1 (-1.32128) | -1 | -1 |
| G: -5311.25950 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.93477 HOMO: -6.41100 LUMO: -0.48980 factor:1 | 1 (-1.30958) | -1 | -1 |
| G: -5311.25950 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.00935 HOMO: -6.52257 LUMO: -0.59865 factor:1 | 1 (-1.38416) | -1 | -1 |
| G: -5311.25950 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.60404 HOMO: -6.63686 LUMO: -0.56055 factor:1 | 1 (-0.97885) | -1 | -1 |
| G: -5311.25950 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.82151 HOMO: -6.79740 LUMO: -0.75376 factor:1 | 1 (-1.19632) | -1 | -1 |
| G: -5311.25950 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.69709 HOMO: -5.89127 LUMO: 0.22313 factor:1 | 1 (-2.07190) | -1 | -1 |
| G: -5311.25950 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11578.51531 HOMO: -6.34842 LUMO: 0.11429 factor:1 | 1 (-2.89012) | -1 | -1 |
| G: -5311.25950 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.89508 HOMO: -6.13617 LUMO: 1.94834 factor:1 | 1 (-2.26989) | -1 | -1 |
| G: -5311.25950 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.93759 HOMO: -6.50080 LUMO: 1.74153 factor:1 | 1 (-2.31240) | -1 | -1 |
| G: -5311.25950 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.63894 HOMO: -6.33481 LUMO: 1.68438 factor:1 | 1 (-2.01375) | -1 | -1 |
| G: -5311.25950 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.71595 HOMO: -6.53073 LUMO: 1.95106 factor:1 | 1 (-2.09076) | -1 | -1 |
| G: -5311.25950 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.60123 HOMO: -6.46270 LUMO: 1.89935 factor:1 | 1 (-1.97604) | -1 | -1 |
| G: -5311.25950 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.75565 HOMO: -5.87222 LUMO: 1.91568 factor:1 | 1 (-2.13046) | -1 | -1 |
| G: -5311.25950 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.65124 HOMO: -6.07630 LUMO: 1.81500 factor:1 | 1 (-2.02605) | -1 | -1 |
| G: -5311.25950 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.98387 HOMO: -6.20964 LUMO: 1.81500 factor:1 | 1 (-2.35868) | -1 | -1 |
| G: -5311.25950 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.89887 HOMO: -6.15522 LUMO: 1.90752 factor:1 | 1 (-1.27368) | -1 | -1 |
| G: -5311.25950 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.09417 HOMO: -6.11984 LUMO: 1.95378 factor:1 | 1 (-1.46898) | -1 | -1 |
| G: -5311.25950 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.98334 HOMO: -6.58516 LUMO: 2.04358 factor:1 | 1 (-1.35815) | -1 | -1 |
| G: -5311.25950 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.03205 HOMO: -7.37156 LUMO: 0.24490 factor:1 | 1 (-1.40686) | 1 | 1 |
| G: -5311.25950 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.01289 HOMO: -6.36474 LUMO: -0.90070 factor:1 | 1 (-1.38770) | -1 | -1 |
| G: -5311.25950 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.98630 HOMO: -6.43549 LUMO: -0.40817 factor:1 | 1 (-1.36111) | -1 | -1 |
| G: -5311.25950 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.23306 HOMO: -7.32258 LUMO: 0.29388 factor:1 | 1 (-1.60787) | 1 | 1 |
| G: -5311.25950 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.17899 HOMO: -6.41372 LUMO: -0.20409 factor:1 | 1 (-1.55380) | -1 | -1 |
| G: -5311.25950 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.77172 HOMO: -7.18381 LUMO: 0.42722 factor:1 | 1 (-1.14652) | 1 | 1 |
| G: -5311.25950 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.86576 HOMO: -6.53890 LUMO: -0.54151 factor:1 | 1 (-1.24057) | -1 | -1 |
| G: -5311.25950 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.77947 HOMO: -6.61509 LUMO: 0.08708 factor:1 | 1 (-1.15428) | -1 | -1 |
| G: -5311.25950 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.99703 HOMO: -6.78108 LUMO: 2.03541 factor:1 | 1 (-1.37183) | -1 | -1 |
| G: -5311.25950 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.72744 HOMO: -6.50896 LUMO: 1.53472 factor:1 | 1 (-1.10225) | -1 | -1 |
| G: -5311.25950 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.03088 HOMO: -6.65591 LUMO: 1.80411 factor:1 | 1 (-1.40569) | -1 | -1 |
| G: -5311.25950 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.98870 HOMO: -6.64502 LUMO: 1.52112 factor:1 | 1 (-1.36351) | -1 | -1 |
| G: -5311.25950 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.95659 HOMO: -6.72938 LUMO: 1.48030 factor:1 | 1 (-1.33140) | -1 | -1 |
| G: -5311.25950 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.06827 HOMO: -6.16882 LUMO: 1.96466 factor:1 | 1 (-1.44307) | -1 | -1 |
| G: -5311.25950 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.91120 HOMO: -6.22597 LUMO: 1.43132 factor:1 | 1 (-1.28601) | -1 | -1 |
| G: -5311.25950 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.25461 HOMO: -6.57699 LUMO: 2.05718 factor:1 | 1 (-1.62942) | -1 | -1 |
| G: -5311.25950 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.89262 HOMO: -6.52529 LUMO: 1.89663 factor:1 | 1 (-1.26742) | -1 | -1 |
| G: -5311.25950 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.63503 HOMO: -6.30760 LUMO: 1.88031 factor:1 | 1 (-1.00984) | -1 | -1 |
| G: -5311.25950 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.90687 HOMO: -6.14977 LUMO: 1.92657 factor:1 | 1 (-1.28168) | -1 | -1 |
| G: -5311.25950 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.69424 HOMO: -6.20964 LUMO: 1.83949 factor:1 | 1 (-1.06905) | -1 | -1 |
| G: -5311.25950 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.97615 HOMO: -6.31848 LUMO: 1.91296 factor:1 | 1 (-1.35096) | -1 | -1 |
| G: -5311.25950 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.05997 HOMO: -5.80691 LUMO: 2.19868 factor:1 | 1 (-1.43477) | -1 | -1 |
| G: -5311.25950 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.75988 HOMO: -6.00827 LUMO: 2.15514 factor:1 | 1 (-1.13469) | -1 | -1 |
| G: -5311.25950 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.98138 HOMO: -6.51713 LUMO: 2.08711 factor:1 | 1 (-1.35619) | -1 | -1 |
| G: -5311.25950 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.89180 HOMO: -6.32937 LUMO: 2.11705 factor:1 | 1 (-1.26661) | -1 | -1 |
| G: -5311.25950 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.85800 HOMO: -6.26678 LUMO: 1.95922 factor:1 | 1 (-1.23281) | -1 | -1 |
| G: -5311.25950 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.76976 HOMO: -6.43005 LUMO: 2.56603 factor:1 | 1 (-1.14457) | -1 | -1 |
| G: -5311.25950 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.49481 HOMO: -6.41644 LUMO: 2.68304 factor:1 | 1 (-0.86962) | -1 | -1 |
| G: -5311.25950 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.62687 HOMO: -5.97834 LUMO: 2.02997 factor:1 | 1 (-1.00168) | -1 | -1 |
| G: -5311.25950 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.54031 HOMO: -6.14161 LUMO: 1.77690 factor:1 | 1 (-0.91512) | -1 | -1 |
| G: -5311.25950 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.89172 HOMO: -6.21508 LUMO: 1.80411 factor:1 | 1 (-1.26653) | -1 | -1 |
| G: -5311.25950 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.98587 HOMO: -6.46270 LUMO: 2.34562 factor:1 | 1 (-1.36068) | -1 | -1 |
| G: -5311.25950 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.88747 HOMO: -6.39195 LUMO: -0.75920 factor:1 | 1 (-1.26228) | -1 | -1 |
| G: -5311.25950 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.07205 HOMO: -7.08584 LUMO: -1.14016 factor:1 | 1 (-1.44686) | -1 | -1 |
| G: -5311.25950 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.73454 HOMO: -6.70216 LUMO: -0.65035 factor:1 | 1 (-1.10935) | -1 | -1 |
| G: -5311.25950 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.13338 HOMO: -6.79468 LUMO: -0.83811 factor:1 | 1 (-1.50819) | -1 | -1 |
| G: -5311.25950 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.00307 HOMO: -6.99877 LUMO: -0.79729 factor:1 | 1 (-1.37788) | -1 | -1 |
| G: -5311.25950 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.07828 HOMO: -7.08040 LUMO: -0.85444 factor:1 | 1 (-1.45309) | -1 | -1 |
| G: -5311.25950 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.34928 HOMO: -7.39333 LUMO: 0.12789 factor:1 | 1 (-1.72409) | 1 | 1 |
| G: -5311.25950 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.16389 HOMO: -7.05047 LUMO: 0.13878 factor:1 | 1 (-1.53870) | -1 | -1 |
| G: -5311.25950 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.98269 HOMO: -6.90897 LUMO: -0.77552 factor:1 | 1 (-1.35749) | -1 | -1 |
| G: -5311.25950 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.92598 HOMO: -7.25456 LUMO: 0.05170 factor:1 | 1 (-1.30079) | 1 | 1 |
| G: -5311.25950 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.99847 HOMO: -6.84638 LUMO: -0.84355 factor:1 | 1 (-1.37328) | -1 | -1 |
| G: -5311.25950 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.17564 HOMO: -6.78108 LUMO: -0.81634 factor:1 | 1 (-1.55045) | -1 | -1 |
| G: -5311.25950 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.10756 HOMO: -6.74570 LUMO: -0.77280 factor:1 | 1 (-1.48237) | -1 | -1 |
| G: -5311.25950 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.14965 HOMO: -7.28177 LUMO: -1.68438 factor:1 | 1 (-1.52446) | -1 | -1 |
| G: -5311.25950 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.28718 HOMO: -7.22190 LUMO: -1.63540 factor:1 | 1 (-1.66199) | -1 | -1 |
| G: -5311.25950 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.83634 HOMO: -7.15932 LUMO: -1.57554 factor:1 | 1 (-1.21115) | -1 | -1 |
| G: -5311.25950 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.87689 HOMO: -6.57971 LUMO: -0.93063 factor:1 | 1 (-1.25170) | -1 | -1 |
| G: -5311.25950 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.76159 HOMO: -6.88176 LUMO: 0.58232 factor:1 | 1 (-1.13640) | -1 | -1 |
| G: -5311.25950 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.96622 HOMO: -6.85727 LUMO: 0.51430 factor:1 | 1 (-1.34103) | -1 | -1 |
| G: -5311.25950 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.91131 HOMO: -6.83550 LUMO: 0.87893 factor:1 | 1 (-1.28612) | -1 | -1 |
| G: -5311.25950 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.75297 HOMO: -7.06680 LUMO: 0.87621 factor:1 | 1 (-1.12778) | 1 | 1 |
| G: -5311.25950 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.09314 HOMO: -6.52257 LUMO: 0.81362 factor:1 | 1 (-1.46795) | -1 | -1 |
| G: -5311.25950 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.01210 HOMO: -6.95523 LUMO: 1.17009 factor:1 | 1 (-1.38691) | -1 | -1 |
| G: -5311.25950 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.00995 HOMO: -7.21374 LUMO: 0.97145 factor:1 | 1 (-1.38476) | 1 | 1 |
| G: -5311.25950 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: -1.54561 factor:1 | 1 (-1.06094) | -1 | -1 |
| G: -5311.25950 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.64532 HOMO: -6.86543 LUMO: -1.52656 factor:1 | 1 (-1.02013) | -1 | -1 |
| G: -5311.25950 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.46450 HOMO: -6.90081 LUMO: -0.78097 factor:1 | 1 (-0.83931) | -1 | -1 |
| G: -5311.25950 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.57027 HOMO: -6.64502 LUMO: -0.82723 factor:1 | 1 (-0.94508) | -1 | -1 |
| G: -5311.25950 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.93199 HOMO: -6.65591 LUMO: -0.82178 factor:1 | 1 (-1.30680) | -1 | -1 |
| G: -5311.25950 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.86516 HOMO: -6.79468 LUMO: -1.46397 factor:1 | 1 (-1.23997) | -1 | -1 |
| G: -5311.25950 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.87806 HOMO: -7.25728 LUMO: 0.73743 factor:1 | 1 (-1.25287) | 1 | -1 |
| G: -5311.25950 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.01920 HOMO: -7.00149 LUMO: 1.30070 factor:1 | 1 (-1.39401) | -1 | -1 |
| G: -5311.25950 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.99382 HOMO: -7.07768 LUMO: 0.78097 factor:1 | 1 (-1.36862) | 1 | -1 |
| G: -5311.25950 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.21148 HOMO: -6.86271 LUMO: 0.86260 factor:1 | 1 (-1.58629) | -1 | -1 |
| G: -5311.25950 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.05012 HOMO: -6.94707 LUMO: 0.39729 factor:1 | 1 (-1.42492) | -1 | -1 |
| G: -5311.25950 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.05969 HOMO: -6.79740 LUMO: 0.67484 factor:1 | 1 (-1.43450) | -1 | -1 |
| G: -5311.25950 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.91713 HOMO: -6.91986 LUMO: -1.14288 factor:1 | 1 (-1.29194) | -1 | -1 |
| G: -5311.25950 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.74649 HOMO: -6.31576 LUMO: 1.01771 factor:1 | 1 (-1.12130) | -1 | -1 |
| G: -5311.25950 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.71291 HOMO: -6.81645 LUMO: 0.81362 factor:1 | 1 (-1.08772) | -1 | -1 |
| G: -5311.25950 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.62253 HOMO: -6.92258 LUMO: -0.99594 factor:1 | 1 (-1.99734) | -1 | -1 |
| G: -5311.25950 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.46533 HOMO: -6.81373 LUMO: 0.61770 factor:1 | 1 (-1.84014) | -1 | -1 |
| G: -5311.25950 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.58476 HOMO: -7.18653 LUMO: 1.19186 factor:1 | 1 (-1.95957) | 1 | 1 |
| G: -5311.25950 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.75299 HOMO: -7.00693 LUMO: 0.45715 factor:1 | 1 (-2.12779) | -1 | -1 |
| G: -5311.25950 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.85318 HOMO: -7.11306 LUMO: 0.53334 factor:1 | 1 (-2.22799) | 1 | 1 |
| G: -5311.25950 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.64346 HOMO: -6.63414 LUMO: -1.64357 factor:1 | 1 (-2.01827) | -1 | -1 |
| G: -5311.25950 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.48506 HOMO: -6.22052 LUMO: -0.74015 factor:1 | 1 (-1.85987) | -1 | -1 |
| G: -5311.25950 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.33309 HOMO: -6.81101 LUMO: -0.50069 factor:1 | 1 (-1.70790) | -1 | -1 |
| G: -5311.25950 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.73184 HOMO: -6.71849 LUMO: -0.51974 factor:1 | 1 (-2.10665) | -1 | -1 |
| G: -5311.25950 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11578.19977 HOMO: -6.72121 LUMO: -1.77690 factor:1 | 1 (-2.57458) | -1 | -1 |
| G: -5311.25950 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11578.08622 HOMO: -6.94162 LUMO: -1.78779 factor:1 | 1 (-2.46102) | -1 | -1 |
| G: -5311.25950 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11578.23781 HOMO: -6.91169 LUMO: 0.88981 factor:1 | 1 (-2.61262) | -1 | -1 |
| G: -5311.25950 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11578.80296 HOMO: -6.97428 LUMO: 0.70750 factor:1 | 1 (-3.17777) | -1 | -1 |
| G: -5311.25950 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11579.10817 HOMO: -6.74842 LUMO: 1.15921 factor:1 | 1 (-3.48298) | -1 | -1 |
| G: -5311.25950 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11578.32276 HOMO: -7.25183 LUMO: -0.99594 factor:1 | 1 (-2.69757) | -1 | -1 |
| G: -5311.25950 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.77533 HOMO: -6.43821 LUMO: -1.00410 factor:1 | 1 (-2.15013) | -1 | -1 |
| G: -5311.25950 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.98591 HOMO: -6.52257 LUMO: -0.68573 factor:1 | 1 (-2.36072) | -1 | -1 |
| G: -5311.25950 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.87840 HOMO: -6.60148 LUMO: -0.52518 factor:1 | 1 (-2.25321) | -1 | -1 |
| G: -5311.25950 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.97277 HOMO: -6.07086 LUMO: -1.39594 factor:1 | 1 (-2.34758) | -1 | -1 |
| G: -5311.25950 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.69840 HOMO: -6.78108 LUMO: -1.54833 factor:1 | 1 (-2.07321) | -1 | -1 |
| G: -5311.25950 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.94856 HOMO: -6.73482 LUMO: -1.01498 factor:1 | 1 (-1.32337) | -1 | -1 |
| G: -5311.25950 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.87166 HOMO: -6.85183 LUMO: 1.06669 factor:1 | 1 (-1.24647) | -1 | -1 |
| G: -5311.25950 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.90965 HOMO: -6.98516 LUMO: 1.43948 factor:1 | 1 (-1.28446) | -1 | -1 |
| G: -5311.25950 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.00655 HOMO: -6.94162 LUMO: 0.79185 factor:1 | 1 (-1.38136) | -1 | -1 |
| G: -5311.25950 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.11714 HOMO: -6.67495 LUMO: -1.06669 factor:1 | 1 (-1.49195) | -1 | -1 |
| G: -5311.25950 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.12220 HOMO: -6.88720 LUMO: -1.00682 factor:1 | 1 (-1.49701) | -1 | -1 |
| G: -5311.25950 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.85648 HOMO: -6.85999 LUMO: -0.78097 factor:1 | 1 (-1.23129) | -1 | -1 |
| G: -5311.25950 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.81740 HOMO: -6.51713 LUMO: -0.89798 factor:1 | 1 (-1.19221) | -1 | -1 |
| G: -5311.25950 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.81618 HOMO: -6.63141 LUMO: -0.91430 factor:1 | 1 (-1.19099) | -1 | -1 |
| G: -5311.25950 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.95885 HOMO: -6.63414 LUMO: 0.04354 factor:1 | 1 (-1.33366) | -1 | -1 |
| G: -5311.25950 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.83052 HOMO: -6.65046 LUMO: -0.73743 factor:1 | 1 (-1.20533) | -1 | -1 |
| G: -5311.25950 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.01050 HOMO: -6.73754 LUMO: -0.71838 factor:1 | 1 (-1.38530) | -1 | -1 |
| G: -5311.25950 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.80295 HOMO: -6.65863 LUMO: -0.60137 factor:1 | 1 (-1.17776) | -1 | -1 |
| G: -5311.25950 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.01471 HOMO: -6.61509 LUMO: -0.47892 factor:1 | 1 (-1.38952) | -1 | -1 |
| G: -5311.25950 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.19855 HOMO: -6.82189 LUMO: -0.64763 factor:1 | 1 (-1.57336) | -1 | -1 |
| G: -5311.25950 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.72736 HOMO: -6.56883 LUMO: -0.51974 factor:1 | 1 (-1.10217) | -1 | -1 |
| G: -5311.25950 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.88973 HOMO: -6.97428 LUMO: -0.95512 factor:1 | 1 (-1.26454) | -1 | -1 |
| G: -5311.25950 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.88704 HOMO: -6.70489 LUMO: -0.04082 factor:1 | 1 (-1.26185) | -1 | -1 |
| G: -5311.25950 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.73245 HOMO: -6.74026 LUMO: 0.02177 factor:1 | 1 (-1.10726) | -1 | -1 |
| G: -5311.25950 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.97768 HOMO: -6.50080 LUMO: -0.89525 factor:1 | 1 (-1.35249) | -1 | -1 |
| G: -5311.25950 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.81076 HOMO: -6.46815 LUMO: -0.61226 factor:1 | 1 (-1.18557) | -1 | -1 |
| G: -5311.25950 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.05297 HOMO: -6.57971 LUMO: -0.64219 factor:1 | 1 (-1.42778) | -1 | -1 |
| G: -5311.25950 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.90119 HOMO: -7.17836 LUMO: 0.37280 factor:1 | 1 (-1.27600) | 1 | 1 |
| G: -5311.25950 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.74421 HOMO: -6.67223 LUMO: 0.12245 factor:1 | 1 (-1.11901) | -1 | -1 |
| G: -5311.25950 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.64317 HOMO: -6.55250 LUMO: 0.22858 factor:1 | 1 (-1.01798) | -1 | -1 |
| G: -5311.25950 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.00709 HOMO: -6.97156 LUMO: -1.12927 factor:1 | 1 (-1.38190) | -1 | -1 |
| G: -5311.25950 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11578.18804 HOMO: -6.78924 LUMO: -0.84900 factor:1 | 1 (-2.56285) | -1 | -1 |
| G: -5311.25950 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11578.94767 HOMO: -6.65046 LUMO: -0.65307 factor:1 | 1 (-3.32248) | -1 | -1 |
| G: -5311.25950 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11578.05460 HOMO: -7.41782 LUMO: 0.08980 factor:1 | 1 (-2.42941) | 1 | 1 |
| G: -5311.25950 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11578.37251 HOMO: -6.56339 LUMO: -0.68573 factor:1 | 1 (-2.74732) | -1 | -1 |
| G: -5311.25950 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11578.11675 HOMO: -6.31032 LUMO: -0.31837 factor:1 | 1 (-2.49156) | -1 | -1 |
| G: -5311.25950 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.80815 HOMO: -6.72938 LUMO: -0.45987 factor:1 | 1 (-1.18296) | -1 | -1 |
| G: -5311.25950 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.66565 HOMO: -6.59876 LUMO: -1.03131 factor:1 | 1 (-1.04045) | -1 | -1 |
| G: -5311.25950 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.82271 HOMO: -7.29265 LUMO: 0.29660 factor:1 | 1 (-1.19752) | 1 | 1 |
| G: -5311.25950 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.76521 HOMO: -6.42189 LUMO: -0.51157 factor:1 | 1 (-1.14002) | -1 | -1 |
| G: -5311.25950 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.98837 HOMO: -6.27767 LUMO: -0.52790 factor:1 | 1 (-1.36318) | -1 | -1 |
| G: -5311.25950 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.71746 HOMO: -6.41644 LUMO: -0.44627 factor:1 | 1 (-1.09227) | -1 | -1 |
| G: -5311.25950 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.72151 HOMO: -6.23413 LUMO: -0.52790 factor:1 | 1 (-1.09632) | -1 | -1 |
| G: -5311.25950 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.47764 HOMO: -6.63414 LUMO: -0.44082 factor:1 | 1 (-0.85245) | -1 | -1 |
| G: -5311.25950 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.97221 HOMO: -7.03142 LUMO: 0.47076 factor:1 | 1 (-1.34702) | -1 | -1 |
| G: -5311.25950 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.79710 HOMO: -6.62053 LUMO: -0.14422 factor:1 | 1 (-2.17190) | -1 | -1 |
| G: -5311.25950 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11578.39194 HOMO: -6.22324 LUMO: 1.96194 factor:1 | 1 (-2.76674) | -1 | -1 |
| G: -5311.25950 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.66313 HOMO: -6.17971 LUMO: 1.71704 factor:1 | 1 (-2.03794) | -1 | -1 |
| G: -5311.25950 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.80635 HOMO: -6.70761 LUMO: 1.68711 factor:1 | 1 (-2.18116) | -1 | -1 |
| G: -5311.25950 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.96902 HOMO: -6.52801 LUMO: 1.56193 factor:1 | 1 (-2.34383) | -1 | -1 |
| G: -5311.25950 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.70898 HOMO: -6.55794 LUMO: 1.52384 factor:1 | 1 (-2.08379) | -1 | -1 |
| G: -5311.25950 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.65320 HOMO: -6.47359 LUMO: 1.82316 factor:1 | 1 (-2.02801) | -1 | -1 |
| G: -5311.25950 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.97879 HOMO: -6.65863 LUMO: 1.83133 factor:1 | 1 (-2.35359) | -1 | -1 |
| G: -5311.25950 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.60357 HOMO: -6.46270 LUMO: 1.90208 factor:1 | 1 (-1.97838) | -1 | -1 |
| G: -5311.25950 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.78003 HOMO: -6.41917 LUMO: 2.03269 factor:1 | 1 (-2.15484) | -1 | -1 |
| G: -5311.25950 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.99318 HOMO: -6.48992 LUMO: 1.87486 factor:1 | 1 (-2.36799) | -1 | -1 |
| G: -5311.25950 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.89133 HOMO: -6.51985 LUMO: 1.69527 factor:1 | 1 (-2.26614) | -1 | -1 |
| G: -5311.25950 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.64357 HOMO: -6.36202 LUMO: 2.05718 factor:1 | 1 (-2.01838) | -1 | -1 |
| G: -5311.25950 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.71337 HOMO: -5.96474 LUMO: 1.88575 factor:1 | 1 (-2.08817) | -1 | -1 |
| G: -5311.25950 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.56610 HOMO: -6.56339 LUMO: 2.04630 factor:1 | 1 (-1.94091) | -1 | -1 |
| G: -5311.25950 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11578.20581 HOMO: -6.43277 LUMO: 1.98371 factor:1 | 1 (-2.58062) | -1 | -1 |
| G: -5311.25950 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11578.78011 HOMO: -6.53345 LUMO: 2.06262 factor:1 | 1 (-3.15492) | -1 | -1 |
| G: -5311.25950 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11578.16317 HOMO: -5.81779 LUMO: 2.11432 factor:1 | 1 (-2.53798) | -1 | -1 |
| G: -5311.25950 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.93772 HOMO: -5.91848 LUMO: 1.86942 factor:1 | 1 (-2.31253) | -1 | -1 |
| G: -5311.25950 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.96855 HOMO: -6.48447 LUMO: 1.70343 factor:1 | 1 (-2.34336) | -1 | -1 |
| G: -5311.25950 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.74956 HOMO: -6.29671 LUMO: -0.89525 factor:1 | 1 (-2.12437) | -1 | -1 |
| G: -5311.25950 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.61415 HOMO: -6.63414 LUMO: -0.76192 factor:1 | 1 (-1.98896) | -1 | -1 |
| G: -5311.25950 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.65117 HOMO: -6.56883 LUMO: -0.86260 factor:1 | 1 (-1.02598) | -1 | -1 |
| G: -5311.25950 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.87381 HOMO: -6.93074 LUMO: -0.27483 factor:1 | 1 (-1.24862) | -1 | -1 |
| G: -5311.25950 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.86274 HOMO: -6.85999 LUMO: -0.01905 factor:1 | 1 (-1.23755) | -1 | -1 |
| G: -5311.25950 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.77433 HOMO: -6.26406 LUMO: 0.21769 factor:1 | 1 (-1.14914) | -1 | -1 |
| G: -5311.25950 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.75863 HOMO: -6.62325 LUMO: 0.31293 factor:1 | 1 (-1.13344) | -1 | -1 |
| G: -5311.25950 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.69073 HOMO: -6.59604 LUMO: 0.19592 factor:1 | 1 (-1.06554) | -1 | -1 |
| G: -5311.25950 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.88622 HOMO: -6.43277 LUMO: -0.27756 factor:1 | 1 (-1.26103) | -1 | -1 |
| G: -5311.25950 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.68766 HOMO: -6.54978 LUMO: -0.46531 factor:1 | 1 (-1.06247) | -1 | -1 |
| G: -5311.25950 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.96815 HOMO: -6.65046 LUMO: -0.15783 factor:1 | 1 (-1.34296) | -1 | -1 |
| G: -5311.25950 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.72434 HOMO: -7.28721 LUMO: 0.23946 factor:1 | 1 (-1.09915) | 1 | 1 |
| G: -5311.25950 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.81936 HOMO: -6.71849 LUMO: -0.56600 factor:1 | 1 (-1.19417) | -1 | -1 |
| G: -5311.25950 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.56866 HOMO: -6.85183 LUMO: -0.84355 factor:1 | 1 (-0.94347) | -1 | -1 |
| G: -5311.25950 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.96481 HOMO: -6.53345 LUMO: -0.84627 factor:1 | 1 (-1.33962) | -1 | -1 |
| G: -5311.25950 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.69520 HOMO: -6.60148 LUMO: -0.63130 factor:1 | 1 (-1.07001) | -1 | -1 |
| G: -5311.25950 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.60766 HOMO: -6.36202 LUMO: -0.60137 factor:1 | 1 (-0.98247) | -1 | -1 |
| G: -5311.25950 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.55049 HOMO: -6.28855 LUMO: -0.52790 factor:1 | 1 (-0.92530) | -1 | -1 |
| G: -5311.25950 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.70728 HOMO: -7.07224 LUMO: 0.41906 factor:1 | 1 (-1.08209) | 1 | 1 |
| G: -5311.25950 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.79612 HOMO: -6.36202 LUMO: -0.24218 factor:1 | 1 (-1.17093) | -1 | -1 |
| G: -5311.25950 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11578.01846 HOMO: -6.43549 LUMO: 0.14150 factor:1 | 1 (-2.39327) | -1 | -1 |
| G: -5311.25950 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11579.11029 HOMO: -6.76747 LUMO: -0.40545 factor:1 | 1 (-3.48510) | -1 | -1 |
| G: -5311.25950 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11578.18981 HOMO: -6.15249 LUMO: -0.51157 factor:1 | 1 (-2.56462) | -1 | -1 |
| G: -5311.25950 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.64992 HOMO: -6.33753 LUMO: -0.02993 factor:1 | 1 (-1.02473) | -1 | -1 |
| G: -5311.25950 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.78140 HOMO: -6.49808 LUMO: -0.83811 factor:1 | 1 (-1.15621) | -1 | -1 |
| G: -5311.25950 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.79923 HOMO: -6.64502 LUMO: -0.46259 factor:1 | 1 (-1.17404) | -1 | -1 |
| G: -5311.25950 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.64826 HOMO: -6.34570 LUMO: 0.22041 factor:1 | 1 (-1.02307) | -1 | -1 |
| G: -5311.25950 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.81841 HOMO: -6.63414 LUMO: -0.13606 factor:1 | 1 (-1.19322) | -1 | -1 |
| G: -5311.25950 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11578.35662 HOMO: -6.59604 LUMO: -0.79729 factor:1 | 1 (-2.73142) | -1 | -1 |
| G: -5311.25950 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.73696 HOMO: -7.09401 LUMO: 0.31837 factor:1 | 1 (-2.11177) | 1 | 1 |
| G: -5311.25950 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.65111 HOMO: -6.48719 LUMO: -0.31021 factor:1 | 1 (-2.02591) | -1 | -1 |
| G: -5311.25950 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.76719 HOMO: -7.11306 LUMO: 0.39729 factor:1 | 1 (-2.14200) | 1 | 1 |
| G: -5311.25950 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.73451 HOMO: -6.95251 LUMO: 0.41089 factor:1 | 1 (-2.10932) | -1 | -1 |
| G: -5311.25950 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.85348 HOMO: -6.61509 LUMO: -0.41906 factor:1 | 1 (-2.22829) | -1 | -1 |
| G: -5311.25950 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11578.54348 HOMO: -6.25318 LUMO: -0.47348 factor:1 | 1 (-2.91829) | -1 | -1 |
| G: -5311.25950 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.61078 HOMO: -6.77019 LUMO: -0.10340 factor:1 | 1 (-1.98559) | -1 | -1 |
| G: -5311.25950 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.94834 HOMO: -6.54706 LUMO: -0.46259 factor:1 | 1 (-1.32315) | -1 | -1 |
| G: -5311.25950 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.11657 HOMO: -6.34297 LUMO: -0.50341 factor:1 | 1 (-1.49137) | -1 | -1 |
| G: -5311.25950 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.05782 HOMO: -6.20692 LUMO: -0.51974 factor:1 | 1 (-1.43263) | -1 | -1 |
| G: -5311.25950 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.05474 HOMO: -7.03686 LUMO: 0.46804 factor:1 | 1 (-1.42955) | -1 | -1 |
| G: -5311.25950 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.01033 HOMO: -6.47087 LUMO: 0.22585 factor:1 | 1 (-1.38514) | -1 | -1 |
| G: -5311.25950 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.11205 HOMO: -6.41917 LUMO: 0.19320 factor:1 | 1 (-1.48686) | -1 | -1 |
| G: -5311.25950 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.89569 HOMO: -6.61237 LUMO: -0.04354 factor:1 | 1 (-1.27050) | -1 | -1 |
| G: -5311.25950 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.76061 HOMO: -6.56339 LUMO: 0.36735 factor:1 | 1 (-1.13542) | -1 | -1 |
| G: -5311.25950 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.28996 HOMO: -6.54978 LUMO: 1.12655 factor:1 | 1 (-1.66477) | -1 | -1 |
| G: -5311.25950 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.12642 HOMO: -6.43277 LUMO: 1.17553 factor:1 | 1 (-1.50122) | -1 | -1 |
| G: -5311.25950 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.16683 HOMO: -6.29944 LUMO: 1.40955 factor:1 | 1 (-1.54163) | -1 | -1 |
| G: -5311.25950 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.12282 HOMO: -6.74842 LUMO: 0.74015 factor:1 | 1 (-1.49763) | -1 | -1 |
| G: -5311.25950 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.26968 HOMO: -6.15522 LUMO: 1.94289 factor:1 | 1 (-1.64449) | -1 | -1 |
| G: -5311.25950 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.27975 HOMO: -6.20147 LUMO: 1.40139 factor:1 | 1 (-1.65456) | -1 | -1 |
| G: -5311.25950 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.99694 HOMO: -6.41100 LUMO: 1.40139 factor:1 | 1 (-1.37175) | -1 | -1 |
| G: -5311.25950 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.02563 HOMO: -6.74570 LUMO: 1.80956 factor:1 | 1 (-1.40043) | -1 | -1 |
| G: -5311.25950 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.49426 HOMO: -6.60148 LUMO: -1.04764 factor:1 | 1 (-1.86907) | -1 | -1 |
| G: -5311.25950 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.27080 HOMO: -6.82734 LUMO: -0.83267 factor:1 | 1 (-1.64561) | -1 | -1 |
| G: -5311.25950 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.21970 HOMO: -7.01782 LUMO: -0.32382 factor:1 | 1 (-1.59451) | -1 | -1 |
| G: -5311.25950 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.41154 HOMO: -6.54434 LUMO: 0.11157 factor:1 | 1 (-1.78635) | -1 | -1 |
| G: -5311.25950 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.12786 HOMO: -6.53617 LUMO: 0.32926 factor:1 | 1 (-1.50267) | -1 | -1 |
| G: -5311.25950 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.03646 HOMO: -6.62597 LUMO: -0.60137 factor:1 | 1 (-1.41126) | -1 | -1 |
| G: -5311.25950 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.04252 HOMO: -6.60965 LUMO: -0.75376 factor:1 | 1 (-1.41733) | -1 | -1 |
| G: -5311.25950 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.17208 HOMO: -6.29399 LUMO: 0.06803 factor:1 | 1 (-1.54689) | -1 | -1 |
| G: -5311.25950 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.27534 HOMO: -6.60692 LUMO: -0.47076 factor:1 | 1 (-1.65015) | -1 | -1 |
| G: -5311.25950 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.19602 HOMO: -7.33891 LUMO: 0.39184 factor:1 | 1 (-1.57083) | 1 | 1 |
| G: -5311.25950 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.34925 HOMO: -6.60692 LUMO: 1.46125 factor:1 | 1 (-1.72406) | -1 | -1 |
| G: -5311.25950 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.23695 HOMO: -6.21780 LUMO: 2.09256 factor:1 | 1 (-1.61176) | -1 | -1 |
| G: -5311.25950 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.24002 HOMO: -6.28311 LUMO: 1.80411 factor:1 | 1 (-1.61483) | -1 | -1 |
| G: -5311.25950 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.05303 HOMO: -6.51168 LUMO: 1.84765 factor:1 | 1 (-1.42784) | -1 | -1 |
| G: -5311.25950 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.00054 HOMO: -6.66951 LUMO: 2.01636 factor:1 | 1 (-1.37535) | -1 | -1 |
| G: -5311.25950 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.78951 HOMO: -6.75387 LUMO: 1.73881 factor:1 | 1 (-1.16432) | -1 | -1 |
| G: -5311.25950 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.03101 HOMO: -6.77291 LUMO: 1.89935 factor:1 | 1 (-1.40582) | -1 | -1 |
| G: -5311.25950 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.20609 HOMO: -6.36474 LUMO: 1.61091 factor:1 | 1 (-1.58090) | -1 | -1 |
| G: -5311.25950 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.03836 HOMO: -6.60420 LUMO: 1.40955 factor:1 | 1 (-1.41317) | -1 | -1 |
| G: -5311.25950 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.91520 HOMO: -6.81645 LUMO: 1.59731 factor:1 | 1 (-1.29001) | -1 | -1 |
| G: -5311.25950 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.18606 HOMO: -5.90215 LUMO: 2.12249 factor:1 | 1 (-1.56087) | -1 | -1 |
| G: -5311.25950 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.73112 HOMO: -6.26950 LUMO: 1.62996 factor:1 | 1 (-1.10593) | -1 | -1 |
| G: -5311.25950 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.61925 HOMO: -6.41100 LUMO: 1.80684 factor:1 | 1 (-0.99406) | -1 | -1 |
| G: -5311.25950 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.08764 HOMO: -6.64230 LUMO: 2.23405 factor:1 | 1 (-1.46245) | -1 | -1 |
| G: -5311.25950 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.22753 HOMO: -6.66951 LUMO: 2.21501 factor:1 | 1 (-1.60234) | -1 | -1 |
| G: -5311.25950 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.01792 HOMO: -6.90897 LUMO: 2.00004 factor:1 | 1 (-1.39273) | -1 | -1 |
| G: -5311.25950 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.30457 HOMO: -6.61781 LUMO: 1.42043 factor:1 | 1 (-1.67938) | -1 | -1 |
| G: -5311.25950 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.11387 HOMO: -6.56611 LUMO: 1.60003 factor:1 | 1 (-1.48868) | -1 | -1 |
| G: -5311.25950 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.87577 HOMO: -6.70489 LUMO: 1.78779 factor:1 | 1 (-1.25058) | -1 | -1 |
| G: -5311.25950 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.67611 HOMO: -6.46815 LUMO: 1.59459 factor:1 | 1 (-2.05092) | -1 | -1 |
| G: -5311.25950 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.67802 HOMO: -6.31304 LUMO: 1.36873 factor:1 | 1 (-2.05283) | -1 | -1 |
| G: -5311.25950 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.99155 HOMO: -6.22597 LUMO: 1.54833 factor:1 | 1 (-2.36636) | -1 | -1 |
| G: -5311.25950 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.90575 HOMO: -5.63004 LUMO: 1.96466 factor:1 | 1 (-2.28056) | -1 | -1 |
| G: -5311.25950 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.85865 HOMO: -7.02598 LUMO: 1.79323 factor:1 | 1 (-2.23346) | -1 | -1 |
| G: -5311.25950 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.81416 HOMO: -6.78924 LUMO: 2.10888 factor:1 | 1 (-2.18897) | -1 | -1 |
| G: -5311.25950 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11578.01541 HOMO: -6.13345 LUMO: 2.07351 factor:1 | 1 (-2.39022) | -1 | -1 |
| G: -5311.25950 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11578.09452 HOMO: -6.46270 LUMO: -0.37552 factor:1 | 1 (-2.46932) | -1 | -1 |
| G: -5311.25950 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.90474 HOMO: -6.51985 LUMO: -0.49525 factor:1 | 1 (-2.27955) | -1 | -1 |
| G: -5311.25950 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.85944 HOMO: -6.60965 LUMO: 1.90480 factor:1 | 1 (-2.23425) | -1 | -1 |
| G: -5311.25950 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.87750 HOMO: -6.51168 LUMO: 1.92112 factor:1 | 1 (-2.25231) | -1 | -1 |
| G: -5311.25950 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.94532 HOMO: -6.71305 LUMO: 1.91024 factor:1 | 1 (-2.32012) | -1 | -1 |
| G: -5311.25950 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.53225 HOMO: -6.86815 LUMO: 2.02997 factor:1 | 1 (-1.90706) | -1 | -1 |
| G: -5311.25950 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.52909 HOMO: -6.69944 LUMO: 1.95106 factor:1 | 1 (-1.90390) | -1 | -1 |
| G: -5311.25950 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.18925 HOMO: -6.45182 LUMO: 1.66806 factor:1 | 1 (-1.56406) | -1 | -1 |
| G: -5311.25950 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.09014 HOMO: -6.44638 LUMO: 2.16058 factor:1 | 1 (-1.46495) | -1 | -1 |
| G: -5311.25950 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.02601 HOMO: -6.65591 LUMO: 1.95106 factor:1 | 1 (-1.40081) | -1 | -1 |
| G: -5311.25950 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.12761 HOMO: -6.35114 LUMO: 1.42316 factor:1 | 1 (-1.50242) | -1 | -1 |
| G: -5311.25950 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.23515 HOMO: -6.48719 LUMO: 1.59187 factor:1 | 1 (-1.60996) | -1 | -1 |
| G: -5311.25950 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.42912 HOMO: -7.05591 LUMO: 1.61908 factor:1 | 1 (-1.80392) | -1 | -1 |
| G: -5311.25950 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.25564 HOMO: -6.92258 LUMO: 1.87214 factor:1 | 1 (-1.63045) | -1 | -1 |
| G: -5311.25950 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.07262 HOMO: -5.85861 LUMO: 2.11705 factor:1 | 1 (-1.44743) | -1 | -1 |
| G: -5311.25950 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.96851 HOMO: -6.27767 LUMO: 1.75513 factor:1 | 1 (-1.34332) | -1 | -1 |
| G: -5311.25950 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.64830 HOMO: -6.16882 LUMO: 1.73881 factor:1 | 1 (-2.02311) | -1 | -1 |
| G: -5311.25950 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.78792 HOMO: -6.62053 LUMO: 1.39594 factor:1 | 1 (-2.16273) | -1 | -1 |
| G: -5311.25950 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.77935 HOMO: -5.46405 LUMO: 1.68166 factor:1 | 1 (-2.15416) | -1 | -1 |
| G: -5311.25950 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.48000 HOMO: -6.39740 LUMO: 1.68711 factor:1 | 1 (-1.85481) | -1 | -1 |
| G: -5311.25950 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.60520 HOMO: -6.99333 LUMO: 2.08439 factor:1 | 1 (-1.98001) | -1 | -1 |
| G: -5311.25950 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.52966 HOMO: -6.16882 LUMO: 1.71976 factor:1 | 1 (-1.90447) | -1 | -1 |
| G: -5311.25950 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.73465 HOMO: -7.19741 LUMO: 2.24766 factor:1 | 1 (-2.10945) | 1 | 1 |
| G: -5311.25950 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.79674 HOMO: -6.77291 LUMO: 2.17691 factor:1 | 1 (-2.17155) | -1 | -1 |
| G: -5311.25950 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.89661 HOMO: -6.29944 LUMO: 2.16603 factor:1 | 1 (-2.27142) | -1 | -1 |
| G: -5311.25950 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.76188 HOMO: -6.10079 LUMO: 1.83949 factor:1 | 1 (-2.13669) | -1 | -1 |
| G: -5311.25950 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.63121 HOMO: -6.63686 LUMO: 2.05990 factor:1 | 1 (-2.00602) | -1 | -1 |
| G: -5311.25950 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.66942 HOMO: -6.91713 LUMO: 1.87486 factor:1 | 1 (-2.04423) | -1 | -1 |
| G: -5311.25950 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.44680 HOMO: -6.63958 LUMO: 1.79323 factor:1 | 1 (-1.82161) | -1 | -1 |
| G: -5311.25950 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.38041 HOMO: -6.61781 LUMO: 1.70071 factor:1 | 1 (-1.75522) | -1 | -1 |
| G: -5311.25950 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.87582 HOMO: -6.20420 LUMO: 1.82861 factor:1 | 1 (-2.25063) | -1 | -1 |
| G: -5311.25950 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.78741 HOMO: -6.47903 LUMO: -2.16875 factor:1 | 1 (-2.16222) | -1 | -1 |
| G: -5311.25950 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.57883 HOMO: -6.53073 LUMO: 2.18235 factor:1 | 1 (-1.95364) | -1 | -1 |
| G: -5311.25950 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.53548 HOMO: -7.01782 LUMO: 1.72520 factor:1 | 1 (-1.91029) | -1 | -1 |
| G: -5311.25950 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.71884 HOMO: -6.66135 LUMO: -0.75648 factor:1 | 1 (-2.09364) | -1 | -1 |
| G: -5311.25950 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.56027 HOMO: -7.56749 LUMO: 0.22585 factor:1 | 1 (-1.93508) | 1 | 1 |
| G: -5311.25950 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.60539 HOMO: -6.45182 LUMO: -0.71294 factor:1 | 1 (-1.98020) | -1 | -1 |
| G: -5311.25950 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.86542 HOMO: -6.31032 LUMO: -0.34286 factor:1 | 1 (-2.24023) | -1 | -1 |
| G: -5311.25950 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.84153 HOMO: -6.41917 LUMO: 2.04085 factor:1 | 1 (-2.21634) | -1 | -1 |
| G: -5311.25950 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.79122 HOMO: -6.61781 LUMO: 1.98915 factor:1 | 1 (-2.16603) | -1 | -1 |
| G: -5311.25950 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.86757 HOMO: -5.86405 LUMO: 1.57282 factor:1 | 1 (-2.24238) | -1 | -1 |
| G: -5311.25950 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.44610 HOMO: -6.44094 LUMO: 1.80956 factor:1 | 1 (-1.82090) | -1 | -1 |
| G: -5311.25950 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.48253 HOMO: -6.59060 LUMO: 2.08167 factor:1 | 1 (-1.85734) | -1 | -1 |
| G: -5311.25950 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11578.00534 HOMO: -6.20147 LUMO: 1.69799 factor:1 | 1 (-2.38015) | -1 | -1 |
| G: -5311.25950 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.02437 HOMO: -6.50352 LUMO: -0.41361 factor:1 | 1 (-1.39918) | -1 | -1 |
| G: -5311.25950 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.83112 HOMO: -6.10896 LUMO: -0.55783 factor:1 | 1 (-1.20593) | -1 | -1 |
| G: -5311.25950 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.03741 HOMO: -6.74842 LUMO: -0.56872 factor:1 | 1 (-1.41222) | -1 | -1 |
| G: -5311.25950 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.16111 HOMO: -6.59060 LUMO: -0.22041 factor:1 | 1 (-1.53592) | -1 | -1 |
| G: -5311.25950 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.77963 HOMO: -6.22052 LUMO: -0.60137 factor:1 | 1 (-1.15444) | -1 | -1 |
| G: -5311.25950 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.97368 HOMO: -6.65863 LUMO: 0.07891 factor:1 | 1 (-1.34849) | -1 | -1 |
| G: -5311.25950 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.91398 HOMO: -6.57427 LUMO: 1.71160 factor:1 | 1 (-1.28879) | -1 | -1 |
| G: -5311.25950 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.86132 HOMO: -5.84773 LUMO: 1.99459 factor:1 | 1 (-1.23613) | -1 | -1 |
| G: -5311.25950 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.74589 HOMO: -6.02188 LUMO: 1.91296 factor:1 | 1 (-1.12070) | -1 | -1 |
| G: -5311.25950 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.68246 HOMO: -6.17698 LUMO: 2.00004 factor:1 | 1 (-1.05727) | -1 | -1 |
| G: -5311.25950 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.05036 HOMO: -6.02732 LUMO: 1.90752 factor:1 | 1 (-1.42517) | -1 | -1 |
| G: -5311.25950 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.90026 HOMO: -6.68584 LUMO: -0.50885 factor:1 | 1 (-1.27507) | -1 | -1 |
| G: -5311.25950 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.29856 HOMO: -6.61781 LUMO: -0.73471 factor:1 | 1 (-1.67336) | -1 | -1 |
| G: -5311.25950 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.01833 HOMO: -6.66407 LUMO: -0.79729 factor:1 | 1 (-1.39314) | -1 | -1 |
| G: -5311.25950 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.92728 HOMO: -6.56339 LUMO: 0.23130 factor:1 | 1 (-1.30209) | -1 | -1 |
| G: -5311.25950 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.89828 HOMO: -6.76747 LUMO: 0.08980 factor:1 | 1 (-1.27308) | -1 | -1 |
| G: -5311.25950 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.85180 HOMO: -6.70489 LUMO: -0.53334 factor:1 | 1 (-1.22661) | -1 | -1 |
| G: -5311.25950 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.98070 HOMO: -7.28993 LUMO: 0.10885 factor:1 | 1 (-1.35551) | 1 | 1 |
| G: -5311.25950 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.20810 HOMO: -6.22052 LUMO: 0.51974 factor:1 | 1 (-1.58291) | -1 | -1 |
| G: -5311.25950 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.69237 HOMO: -6.81645 LUMO: 0.25307 factor:1 | 1 (-1.06718) | -1 | -1 |
| G: -5311.25950 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.96824 HOMO: -6.80285 LUMO: 0.02721 factor:1 | 1 (-1.34305) | -1 | -1 |
| G: -5311.25950 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.09997 HOMO: -6.51441 LUMO: 0.08163 factor:1 | 1 (-1.47478) | -1 | -1 |
| G: -5311.25950 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.91844 HOMO: -6.73482 LUMO: -0.77008 factor:1 | 1 (-1.29325) | -1 | -1 |
| G: -5311.25950 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.90443 HOMO: -6.29127 LUMO: -0.44355 factor:1 | 1 (-1.27923) | -1 | -1 |
| G: -5311.25950 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.82214 HOMO: -6.72938 LUMO: -0.64763 factor:1 | 1 (-1.19695) | -1 | -1 |
| G: -5311.25950 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.06573 HOMO: -6.49264 LUMO: -0.74559 factor:1 | 1 (-1.44054) | -1 | -1 |
| G: -5311.25950 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.81558 HOMO: -6.67223 LUMO: -0.55239 factor:1 | 1 (-1.19039) | -1 | -1 |
| G: -5311.25950 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.76570 HOMO: -6.33481 LUMO: 0.33198 factor:1 | 1 (-1.14051) | -1 | -1 |
| G: -5311.25950 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.68400 HOMO: -6.76475 LUMO: -0.25307 factor:1 | 1 (-2.05881) | -1 | -1 |
| G: -5311.25950 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.88300 HOMO: -6.65318 LUMO: 0.03810 factor:1 | 1 (-2.25781) | -1 | -1 |
| G: -5311.25950 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.80422 HOMO: -6.09263 LUMO: 0.21497 factor:1 | 1 (-2.17903) | -1 | -1 |
| G: -5311.25950 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.33064 HOMO: -6.32120 LUMO: -0.85444 factor:1 | 1 (-1.70545) | -1 | -1 |
| G: -5311.25950 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.75894 HOMO: -6.57155 LUMO: -0.67484 factor:1 | 1 (-2.13375) | -1 | -1 |
| G: -5311.25950 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.47532 HOMO: -6.53345 LUMO: -0.78913 factor:1 | 1 (-1.85013) | -1 | -1 |
| G: -5311.25950 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.45513 HOMO: -7.07768 LUMO: 0.28844 factor:1 | 1 (-1.82994) | 1 | 1 |
| G: -5311.25950 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.65290 HOMO: -6.75114 LUMO: 0.18776 factor:1 | 1 (-2.02771) | -1 | -1 |
| G: -5311.25950 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.93150 HOMO: -6.77019 LUMO: -0.12245 factor:1 | 1 (-1.30631) | -1 | -1 |
| G: -5311.25950 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.92059 HOMO: -6.43549 LUMO: 0.16327 factor:1 | 1 (-1.29540) | -1 | -1 |
| G: -5311.25950 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.20541 HOMO: -6.69400 LUMO: -0.16327 factor:1 | 1 (-1.58022) | -1 | -1 |
| G: -5311.25950 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.73593 HOMO: -6.38651 LUMO: -0.61770 factor:1 | 1 (-1.11074) | -1 | -1 |
| G: -5311.25950 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.74094 HOMO: -6.34297 LUMO: -0.33198 factor:1 | 1 (-1.11575) | -1 | -1 |
| G: -5311.25950 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.04489 HOMO: -7.51578 LUMO: 0.02177 factor:1 | 1 (-1.41970) | 1 | 1 |
| G: -5311.25950 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.92568 HOMO: -6.47359 LUMO: -0.22585 factor:1 | 1 (-1.30049) | -1 | -1 |
| G: -5311.25950 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.98187 HOMO: -6.68040 LUMO: -0.47076 factor:1 | 1 (-1.35668) | -1 | -1 |
| G: -5311.25950 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.27722 HOMO: -6.75659 LUMO: -0.57688 factor:1 | 1 (-1.65203) | -1 | -1 |
| G: -5311.25950 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.82358 HOMO: -6.73754 LUMO: -0.61226 factor:1 | 1 (-1.19839) | -1 | -1 |
| G: -5311.25950 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.57054 HOMO: -7.37429 LUMO: 0.31293 factor:1 | 1 (-0.94535) | 1 | 1 |
| G: -5311.25950 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.08184 HOMO: -6.23413 LUMO: -0.90886 factor:1 | 1 (-1.45665) | -1 | -1 |
| G: -5311.25950 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.70129 HOMO: -6.51985 LUMO: -0.68028 factor:1 | 1 (-1.07610) | -1 | -1 |
| G: -5311.25950 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.94511 HOMO: -6.52257 LUMO: -0.77280 factor:1 | 1 (-1.31992) | -1 | -1 |
| G: -5311.25950 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.06628 HOMO: -7.29537 LUMO: 0.31837 factor:1 | 1 (-1.44109) | 1 | 1 |
| G: -5311.25950 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.78309 HOMO: -6.08447 LUMO: 0.25851 factor:1 | 1 (-1.15790) | -1 | -1 |
| G: -5311.25950 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.83762 HOMO: -6.20964 LUMO: 0.13606 factor:1 | 1 (-1.21243) | -1 | -1 |
| G: -5311.25950 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.66676 HOMO: -6.49808 LUMO: -0.14150 factor:1 | 1 (-1.04157) | -1 | -1 |
| G: -5311.25950 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.03112 HOMO: -7.10761 LUMO: 0.28028 factor:1 | 1 (-1.40593) | 1 | 1 |
| G: -5311.25950 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.22819 HOMO: -6.60965 LUMO: -0.62858 factor:1 | 1 (-1.60300) | -1 | -1 |
| G: -5311.25950 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.85466 HOMO: -6.40012 LUMO: -0.26939 factor:1 | 1 (-1.22946) | -1 | -1 |
| G: -5311.25950 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.01031 HOMO: -6.65318 LUMO: -0.73199 factor:1 | 1 (-1.38511) | -1 | -1 |
| G: -5311.25950 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.97088 HOMO: -6.51441 LUMO: -0.44899 factor:1 | 1 (-1.34568) | -1 | -1 |
| G: -5311.25950 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.19308 HOMO: -6.28583 LUMO: -0.48708 factor:1 | 1 (-1.56789) | -1 | -1 |
| G: -5311.25950 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.08269 HOMO: -6.96884 LUMO: 0.19864 factor:1 | 1 (-1.45750) | -1 | -1 |
| G: -5311.25950 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.92135 HOMO: -6.89809 LUMO: 0.34558 factor:1 | 1 (-1.29616) | -1 | -1 |
| G: -5311.25950 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.92456 HOMO: -6.67495 LUMO: -0.15510 factor:1 | 1 (-1.29937) | -1 | -1 |
| G: -5311.25950 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.84701 HOMO: -7.34980 LUMO: 0.19864 factor:1 | 1 (-1.22182) | 1 | 1 |
| G: -5311.25950 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.89330 HOMO: -6.71305 LUMO: -0.81634 factor:1 | 1 (-1.26811) | -1 | -1 |
| G: -5311.25950 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.72197 HOMO: -6.39468 LUMO: -0.47076 factor:1 | 1 (-1.09678) | -1 | -1 |
| G: -5311.25950 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.94451 HOMO: -6.31304 LUMO: 1.39594 factor:1 | 1 (-1.31932) | -1 | -1 |
| G: -5311.25950 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.79626 HOMO: -6.57155 LUMO: 1.55105 factor:1 | 1 (-1.17107) | -1 | -1 |
| G: -5311.25950 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.07939 HOMO: -6.68312 LUMO: 1.69255 factor:1 | 1 (-1.45420) | -1 | -1 |
| G: -5311.25950 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.96478 HOMO: -6.61509 LUMO: 1.73881 factor:1 | 1 (-1.33959) | -1 | -1 |
| G: -5311.25950 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.76636 HOMO: -6.17971 LUMO: 1.90208 factor:1 | 1 (-1.14116) | -1 | -1 |
| G: -5311.25950 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.13714 HOMO: -6.53073 LUMO: 1.73337 factor:1 | 1 (-1.51195) | -1 | -1 |
| G: -5311.25950 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.75381 HOMO: -5.91303 LUMO: 1.90480 factor:1 | 1 (-1.12862) | -1 | -1 |
| G: -5311.25950 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.68619 HOMO: -6.42733 LUMO: 1.80139 factor:1 | 1 (-1.06100) | -1 | -1 |
| G: -5311.25950 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.49944 HOMO: -6.78924 LUMO: 2.31569 factor:1 | 1 (-0.87425) | -1 | -1 |
| G: -5311.25950 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.92116 HOMO: -6.04093 LUMO: 1.91568 factor:1 | 1 (-1.29597) | -1 | -1 |
| G: -5311.25950 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.03504 HOMO: -6.90081 LUMO: 2.36739 factor:1 | 1 (-1.40985) | -1 | -1 |
| G: -5311.25950 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.07667 HOMO: -6.60965 LUMO: 2.18507 factor:1 | 1 (-1.45148) | -1 | -1 |
| G: -5311.25950 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.74293 HOMO: -6.75387 LUMO: 2.48712 factor:1 | 1 (-1.11773) | -1 | -1 |
| G: -5311.25950 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.64899 HOMO: -6.56883 LUMO: 1.71432 factor:1 | 1 (-1.02380) | -1 | -1 |
| G: -5311.25950 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.11213 HOMO: -6.41644 LUMO: 1.72792 factor:1 | 1 (-1.48694) | -1 | -1 |
| G: -5311.25950 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.13232 HOMO: -6.92530 LUMO: 2.54426 factor:1 | 1 (-1.50713) | -1 | -1 |
| G: -5311.25950 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.21714 HOMO: -6.41644 LUMO: 2.70209 factor:1 | 1 (-1.59195) | -1 | -1 |
| G: -5311.25950 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.27488 HOMO: -6.29671 LUMO: 2.14698 factor:1 | 1 (-1.64969) | -1 | -1 |
| G: -5311.25950 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.01229 HOMO: -6.29127 LUMO: 1.87486 factor:1 | 1 (-1.38710) | -1 | -1 |
| G: -5311.25950 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.12990 HOMO: -6.75931 LUMO: 2.78917 factor:1 | 1 (-1.50471) | -1 | -1 |
| G: -5311.25950 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.98062 HOMO: -6.40828 LUMO: 1.86942 factor:1 | 1 (-1.35543) | -1 | -1 |
| G: -5311.25950 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.63745 HOMO: -6.45726 LUMO: 1.97010 factor:1 | 1 (-2.01225) | -1 | -1 |
| G: -5311.25950 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.52874 HOMO: -6.43277 LUMO: 1.22723 factor:1 | 1 (-1.90355) | -1 | -1 |
| G: -5311.25950 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.70515 HOMO: -6.63414 LUMO: 1.62452 factor:1 | 1 (-2.07996) | -1 | -1 |
| G: -5311.25950 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.89748 HOMO: -6.54162 LUMO: 2.16058 factor:1 | 1 (-2.27229) | -1 | -1 |
| G: -5311.25950 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.57842 HOMO: -6.40284 LUMO: 1.88575 factor:1 | 1 (-1.95323) | -1 | -1 |
| G: -5311.25950 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.45472 HOMO: -6.20964 LUMO: 1.84221 factor:1 | 1 (-1.82953) | -1 | -1 |
| G: -5311.25950 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.96644 HOMO: -6.58516 LUMO: 1.69799 factor:1 | 1 (-1.34125) | -1 | -1 |
| G: -5311.25950 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.98712 HOMO: -6.44094 LUMO: 2.05446 factor:1 | 1 (-1.36193) | -1 | -1 |
| G: -5311.25950 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.79120 HOMO: -6.61509 LUMO: 2.16058 factor:1 | 1 (-1.16601) | -1 | -1 |
| G: -5311.25950 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.68412 HOMO: -6.65591 LUMO: 1.69527 factor:1 | 1 (-1.05893) | -1 | -1 |
| G: -5311.25950 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.41359 HOMO: -5.55112 LUMO: 1.80411 factor:1 | 1 (-0.78840) | -1 | -1 |
| G: -5311.25950 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.86970 HOMO: -6.68312 LUMO: 2.38100 factor:1 | 1 (-1.24451) | -1 | -1 |
| G: -5311.25950 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.60431 HOMO: -6.51168 LUMO: 2.14698 factor:1 | 1 (-0.97912) | -1 | -1 |
| G: -5311.25950 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.29957 HOMO: -6.04637 LUMO: 1.48302 factor:1 | 1 (-0.67438) | -1 | -1 |
| G: -5311.25950 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.16326 HOMO: -6.81645 LUMO: -0.74287 factor:1 | 1 (-1.53807) | -1 | -1 |
| G: -5311.25950 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.08745 HOMO: -6.96884 LUMO: -0.97961 factor:1 | 1 (-1.46226) | -1 | -1 |
| G: -5311.25950 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.26451 HOMO: -6.45998 LUMO: 0.09796 factor:1 | 1 (-1.63932) | -1 | -1 |
| G: -5311.25950 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.38332 HOMO: -6.44638 LUMO: 0.09524 factor:1 | 1 (-1.75813) | -1 | -1 |
| G: -5311.25950 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.39948 HOMO: -6.16338 LUMO: -0.54151 factor:1 | 1 (-1.77429) | -1 | -1 |
| G: -5311.25950 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.03632 HOMO: -6.35930 LUMO: -0.47892 factor:1 | 1 (-1.41113) | -1 | -1 |
| G: -5311.25950 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.09812 HOMO: -6.65318 LUMO: -0.00272 factor:1 | 1 (-1.47293) | -1 | -1 |
| G: -5311.25950 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.94685 HOMO: -6.50080 LUMO: 0.14694 factor:1 | 1 (-1.32166) | -1 | -1 |
| G: -5311.25950 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.28601 HOMO: -6.60420 LUMO: 0.94968 factor:1 | 1 (-1.66082) | -1 | -1 |
| G: -5311.25950 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.99713 HOMO: -6.60148 LUMO: -0.77552 factor:1 | 1 (-1.37194) | -1 | -1 |
| G: -5311.25950 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.09074 HOMO: -6.81645 LUMO: -1.05580 factor:1 | 1 (-1.46555) | -1 | -1 |
| G: -5311.25950 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.34656 HOMO: -6.57971 LUMO: -0.82178 factor:1 | 1 (-1.72137) | -1 | -1 |
| G: -5311.25950 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.19115 HOMO: -6.09263 LUMO: -0.45171 factor:1 | 1 (-1.56596) | -1 | -1 |
| G: -5311.25950 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.84086 HOMO: -6.74298 LUMO: -0.61770 factor:1 | 1 (-1.21567) | -1 | -1 |
| G: -5311.25950 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.68709 HOMO: -6.72393 LUMO: 1.21091 factor:1 | 1 (-1.06190) | -1 | -1 |
| G: -5311.25950 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.80132 HOMO: -6.30488 LUMO: 1.70071 factor:1 | 1 (-1.17613) | -1 | -1 |
| G: -5311.25950 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.69625 HOMO: -6.38107 LUMO: 1.55649 factor:1 | 1 (-2.07106) | -1 | -1 |
| G: -5311.25950 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.81827 HOMO: -6.17154 LUMO: 1.46669 factor:1 | 1 (-2.19307) | -1 | -1 |
| G: -5311.25950 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.88526 HOMO: -6.86543 LUMO: 1.98643 factor:1 | 1 (-2.26007) | -1 | -1 |
| G: -5311.25950 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.88980 HOMO: -6.69944 LUMO: 1.65173 factor:1 | 1 (-2.26461) | -1 | -1 |
| G: -5311.25950 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11578.06652 HOMO: -6.77836 LUMO: 2.16331 factor:1 | 1 (-2.44132) | -1 | -1 |
| G: -5311.25950 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.83829 HOMO: -6.42189 LUMO: 2.36467 factor:1 | 1 (-2.21310) | -1 | -1 |
| G: -5311.25950 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.65535 HOMO: -7.00965 LUMO: 2.04358 factor:1 | 1 (-2.03016) | -1 | -1 |
| G: -5311.25950 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.04835 HOMO: -6.36746 LUMO: 2.13881 factor:1 | 1 (-1.42316) | -1 | -1 |
| G: -5311.25950 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.15640 HOMO: -6.37835 LUMO: 1.89935 factor:1 | 1 (-1.53121) | -1 | -1 |
| G: -5311.25950 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.17488 HOMO: -7.03959 LUMO: 1.27349 factor:1 | 1 (-1.54969) | -1 | -1 |
| G: -5311.25950 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.31189 HOMO: -6.67495 LUMO: -0.89253 factor:1 | 1 (-1.68670) | -1 | -1 |
| G: -5311.25950 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.35012 HOMO: -6.71849 LUMO: -0.97961 factor:1 | 1 (-1.72493) | -1 | -1 |
| G: -5311.25950 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.09091 HOMO: -6.47903 LUMO: 0.01633 factor:1 | 1 (-1.46571) | -1 | -1 |
| G: -5311.25950 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.99406 HOMO: -6.38379 LUMO: 0.01088 factor:1 | 1 (-1.36887) | -1 | -1 |
| G: -5311.25950 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.75104 HOMO: -6.49536 LUMO: -0.55239 factor:1 | 1 (-1.12584) | -1 | -1 |
| G: -5311.25950 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.06114 HOMO: -6.53345 LUMO: -0.53879 factor:1 | 1 (-1.43594) | -1 | -1 |
| G: -5311.25950 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.94192 HOMO: -6.16610 LUMO: 2.15514 factor:1 | 1 (-1.31673) | -1 | -1 |
| G: -5311.25950 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.88837 HOMO: -6.35114 LUMO: 1.98643 factor:1 | 1 (-1.26318) | -1 | -1 |
| G: -5311.25950 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.07659 HOMO: -6.43277 LUMO: 2.16058 factor:1 | 1 (-1.45140) | -1 | -1 |
| G: -5311.25950 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.91991 HOMO: -6.89809 LUMO: 2.20684 factor:1 | 1 (-1.29472) | -1 | -1 |
| G: -5311.25950 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.06304 HOMO: -6.54434 LUMO: 1.93473 factor:1 | 1 (-1.43785) | -1 | -1 |
| G: -5311.25950 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.96138 HOMO: -6.72938 LUMO: 2.03269 factor:1 | 1 (-1.33619) | -1 | -1 |
| G: -5311.25950 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.70750 HOMO: -6.90353 LUMO: 2.19868 factor:1 | 1 (-1.08231) | -1 | -1 |
| G: -5311.25950 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.84739 HOMO: -6.41372 LUMO: 2.02453 factor:1 | 1 (-1.22220) | -1 | -1 |
| G: -5311.25950 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.58676 HOMO: -6.46543 LUMO: 1.90752 factor:1 | 1 (-0.96157) | -1 | -1 |
| G: -5311.25950 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.81666 HOMO: -6.55522 LUMO: 2.11977 factor:1 | 1 (-2.19147) | -1 | -1 |
| G: -5311.25950 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.73437 HOMO: -6.28855 LUMO: 2.02181 factor:1 | 1 (-2.10918) | -1 | -1 |
| G: -5311.25950 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.79914 HOMO: -6.45726 LUMO: 1.52112 factor:1 | 1 (-2.17394) | -1 | -1 |
| G: -5311.25950 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.63399 HOMO: -6.37291 LUMO: 2.11705 factor:1 | 1 (-2.00880) | -1 | -1 |
| G: -5311.25950 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.89179 HOMO: -6.88448 LUMO: 2.24494 factor:1 | 1 (-2.26660) | -1 | -1 |
| G: -5311.25950 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.87125 HOMO: -6.86271 LUMO: 2.41637 factor:1 | 1 (-2.24606) | -1 | -1 |
| G: -5311.25950 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11578.06064 HOMO: -6.69400 LUMO: 2.34562 factor:1 | 1 (-2.43545) | -1 | -1 |
| G: -5311.25950 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.61208 HOMO: -6.18243 LUMO: 2.53882 factor:1 | 1 (-1.98689) | -1 | -1 |
| G: -5311.25950 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.62373 HOMO: -6.61237 LUMO: 2.54154 factor:1 | 1 (-1.99854) | -1 | -1 |
| G: -5311.25950 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.53227 HOMO: -6.69672 LUMO: 2.16331 factor:1 | 1 (-1.90708) | -1 | -1 |
| G: -5311.25950 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.94232 HOMO: -6.33481 LUMO: 2.34018 factor:1 | 1 (-2.31713) | -1 | -1 |
| G: -5311.25950 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.12125 HOMO: -5.99739 LUMO: 2.37283 factor:1 | 1 (-1.49605) | -1 | -1 |
| G: -5311.25950 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.03354 HOMO: -6.49808 LUMO: 2.47351 factor:1 | 1 (-1.40835) | -1 | -1 |
| G: -5311.25950 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.34838 HOMO: -6.22052 LUMO: 1.86398 factor:1 | 1 (-1.72319) | -1 | -1 |
| G: -5311.25950 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.90081 HOMO: -6.32665 LUMO: 2.28031 factor:1 | 1 (-1.27562) | -1 | -1 |
| G: -5311.25950 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.73860 HOMO: -5.98378 LUMO: 2.16331 factor:1 | 1 (-1.11341) | -1 | -1 |
| G: -5311.25950 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.93972 HOMO: -6.08991 LUMO: 2.30208 factor:1 | 1 (-1.31453) | -1 | -1 |
| G: -5311.25950 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.95477 HOMO: -7.07224 LUMO: 1.55105 factor:1 | 1 (-1.32958) | 1 | 1 |
| G: -5311.25950 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.23238 HOMO: -6.84638 LUMO: 1.76874 factor:1 | 1 (-1.60719) | -1 | -1 |
| G: -5311.25950 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.09940 HOMO: -6.68856 LUMO: 1.47758 factor:1 | 1 (-1.47420) | -1 | -1 |
| G: -5311.25950 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.70935 HOMO: -6.69672 LUMO: 1.71976 factor:1 | 1 (-1.08416) | -1 | -1 |
| G: -5311.25950 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.63765 HOMO: -6.86543 LUMO: 2.24766 factor:1 | 1 (-1.01245) | -1 | -1 |
| G: -5311.25950 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.10530 HOMO: -7.21646 LUMO: 1.71976 factor:1 | 1 (-1.48011) | 1 | 1 |
| G: -5311.25950 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.99441 HOMO: -6.94162 LUMO: 2.21773 factor:1 | 1 (-1.36922) | -1 | -1 |
| G: -5311.25950 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.93267 HOMO: -6.34842 LUMO: 2.04358 factor:1 | 1 (-1.30748) | -1 | -1 |
| G: -5311.25950 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.20152 HOMO: -6.53345 LUMO: 1.96738 factor:1 | 1 (-1.57633) | -1 | -1 |
| G: -5311.25950 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.25621 HOMO: -6.34842 LUMO: 1.88303 factor:1 | 1 (-1.63102) | -1 | -1 |
| G: -5311.25950 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.79329 HOMO: -6.38651 LUMO: 2.08983 factor:1 | 1 (-1.16810) | -1 | -1 |
| G: -5311.25950 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.80742 HOMO: -6.01372 LUMO: 1.43676 factor:1 | 1 (-1.18223) | -1 | -1 |
| G: -5311.25950 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.01920 HOMO: -6.30216 LUMO: 1.41771 factor:1 | 1 (-1.39401) | -1 | -1 |
| G: -5311.25950 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.68891 HOMO: -6.52801 LUMO: 1.77146 factor:1 | 1 (-1.06372) | -1 | -1 |
| G: -5311.25950 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.49084 HOMO: -6.53617 LUMO: 1.72792 factor:1 | 1 (-0.86565) | -1 | -1 |
| G: -5311.25950 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.67669 HOMO: -6.56611 LUMO: 2.20412 factor:1 | 1 (-1.05150) | -1 | -1 |
| G: -5311.25950 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.59922 HOMO: -6.66679 LUMO: -0.72927 factor:1 | 1 (-0.97403) | -1 | -1 |
| G: -5311.25950 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.93433 HOMO: -6.85455 LUMO: -0.85444 factor:1 | 1 (-1.30914) | -1 | -1 |
| G: -5311.25950 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.64290 HOMO: -7.21646 LUMO: 0.27211 factor:1 | 1 (-1.01771) | 1 | 1 |
| G: -5311.25950 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.13787 HOMO: -6.57971 LUMO: -0.41361 factor:1 | 1 (-1.51268) | -1 | -1 |
| G: -5311.25950 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.85610 HOMO: -7.03142 LUMO: -1.14288 factor:1 | 1 (-1.23091) | -1 | -1 |
| G: -5311.25950 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.02211 HOMO: -6.29944 LUMO: 0.06803 factor:1 | 1 (-1.39692) | -1 | -1 |
| G: -5311.25950 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.09765 HOMO: -6.47359 LUMO: 0.28028 factor:1 | 1 (-1.47246) | -1 | -1 |
| G: -5311.25950 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.72420 HOMO: -6.42189 LUMO: 1.61364 factor:1 | 1 (-1.09901) | -1 | -1 |
| G: -5311.25950 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.97920 HOMO: -6.41100 LUMO: 1.80956 factor:1 | 1 (-1.35401) | -1 | -1 |
| G: -5311.25950 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.78480 HOMO: -6.83278 LUMO: 1.83949 factor:1 | 1 (-1.15961) | -1 | -1 |
| G: -5311.25950 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.86992 HOMO: -6.78380 LUMO: -0.76192 factor:1 | 1 (-1.24473) | -1 | -1 |
| G: -5311.25950 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.14786 HOMO: -6.95795 LUMO: 2.13609 factor:1 | 1 (-1.52267) | -1 | -1 |
| G: -5311.25950 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.73572 HOMO: -6.57155 LUMO: 1.89119 factor:1 | 1 (-1.11052) | -1 | -1 |
| G: -5311.25950 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.45800 HOMO: -6.65591 LUMO: 1.93745 factor:1 | 1 (-0.83280) | -1 | -1 |
| G: -5311.25950 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.77854 HOMO: -6.44638 LUMO: 2.26943 factor:1 | 1 (-2.15335) | -1 | -1 |
| G: -5311.25950 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.95933 HOMO: -5.88038 LUMO: 1.90480 factor:1 | 1 (-2.33414) | -1 | -1 |
| G: -5311.25950 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.75620 HOMO: -6.22052 LUMO: 2.17691 factor:1 | 1 (-2.13101) | -1 | -1 |
| G: -5311.25950 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.81748 HOMO: -6.04637 LUMO: 2.23950 factor:1 | 1 (-2.19229) | -1 | -1 |
| G: -5311.25950 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.87786 HOMO: -6.44366 LUMO: 2.24766 factor:1 | 1 (-2.25267) | -1 | -1 |
| G: -5311.25950 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11578.09582 HOMO: -6.81917 LUMO: 2.08439 factor:1 | 1 (-2.47063) | -1 | -1 |
| G: -5311.25950 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11578.06219 HOMO: -6.48447 LUMO: 2.28576 factor:1 | 1 (-2.43700) | -1 | -1 |
| G: -5311.25950 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.79258 HOMO: -6.54434 LUMO: 1.99187 factor:1 | 1 (-2.16739) | -1 | -1 |
| G: -5311.25950 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.97930 HOMO: -6.17698 LUMO: -0.65852 factor:1 | 1 (-2.35411) | -1 | -1 |
| G: -5311.25950 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.65464 HOMO: -6.08174 LUMO: -0.58504 factor:1 | 1 (-2.02945) | -1 | -1 |
| G: -5311.25950 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.59236 HOMO: -6.55250 LUMO: -0.86804 factor:1 | 1 (-1.96717) | -1 | -1 |
| G: -5311.25950 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.58583 HOMO: -6.57699 LUMO: -0.89525 factor:1 | 1 (-1.96063) | -1 | -1 |
| G: -5311.25950 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.70866 HOMO: -6.63141 LUMO: -1.04220 factor:1 | 1 (-2.08347) | -1 | -1 |
| G: -5311.25950 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.61007 HOMO: -6.69128 LUMO: -0.76736 factor:1 | 1 (-1.98488) | -1 | -1 |
| G: -5311.25950 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.45736 HOMO: -6.25318 LUMO: -1.03131 factor:1 | 1 (-1.83217) | -1 | -1 |
| G: -5311.25950 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.84159 HOMO: -6.69944 LUMO: 0.01905 factor:1 | 1 (-2.21639) | -1 | -1 |
| G: -5311.25950 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.73775 HOMO: -6.28583 LUMO: 0.38368 factor:1 | 1 (-2.11256) | -1 | -1 |
| G: -5311.25950 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.76866 HOMO: -6.90081 LUMO: -0.83811 factor:1 | 1 (-2.14347) | -1 | -1 |
| G: -5311.25950 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.69198 HOMO: -6.78380 LUMO: -0.10068 factor:1 | 1 (-2.06679) | -1 | -1 |
| G: -5311.25950 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.64398 HOMO: -6.30488 LUMO: -0.98505 factor:1 | 1 (-2.01879) | -1 | -1 |
| G: -5311.25950 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.45382 HOMO: -6.29671 LUMO: -1.79051 factor:1 | 1 (-1.82863) | -1 | -1 |
| G: -5311.25950 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.45067 HOMO: -6.76747 LUMO: -0.22041 factor:1 | 1 (-1.82548) | -1 | -1 |
| G: -5311.25950 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.73813 HOMO: -6.22597 LUMO: -0.94968 factor:1 | 1 (-2.11294) | -1 | -1 |
| G: -5311.25950 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.61706 HOMO: -6.73482 LUMO: 0.05987 factor:1 | 1 (-1.99187) | -1 | -1 |
| G: -5311.25950 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.77612 HOMO: -6.28855 LUMO: 0.34831 factor:1 | 1 (-2.15092) | -1 | -1 |
| G: -5311.25950 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.90036 HOMO: -6.69400 LUMO: 0.25307 factor:1 | 1 (-2.27517) | -1 | -1 |
| G: -5311.25950 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.63804 HOMO: -6.70216 LUMO: 0.61226 factor:1 | 1 (-2.01285) | -1 | -1 |
| G: -5311.25950 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.69415 HOMO: -6.70216 LUMO: 0.17415 factor:1 | 1 (-2.06896) | -1 | -1 |
| G: -5311.25950 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.90746 HOMO: -6.70761 LUMO: 0.24762 factor:1 | 1 (-2.28227) | -1 | -1 |
| G: -5311.25950 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.72390 HOMO: -6.68856 LUMO: -0.84900 factor:1 | 1 (-2.09871) | -1 | -1 |
| G: -5311.25950 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.56887 HOMO: -6.71033 LUMO: -0.38640 factor:1 | 1 (-1.94368) | -1 | -1 |
| G: -5311.25950 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.67791 HOMO: -6.24501 LUMO: -0.09252 factor:1 | 1 (-2.05272) | -1 | -1 |
| G: -5311.25950 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.82305 HOMO: -6.81645 LUMO: -0.07347 factor:1 | 1 (-2.19786) | -1 | -1 |
| G: -5311.25950 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.67788 HOMO: -6.49536 LUMO: 0.09796 factor:1 | 1 (-2.05269) | -1 | -1 |
| G: -5311.25950 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.51148 HOMO: -6.71033 LUMO: -0.26395 factor:1 | 1 (-1.88629) | -1 | -1 |
| G: -5311.25950 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.85220 HOMO: -6.70489 LUMO: -0.09252 factor:1 | 1 (-2.22701) | -1 | -1 |
| G: -5311.25950 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.90191 HOMO: -6.23685 LUMO: 0.39729 factor:1 | 1 (-2.27672) | -1 | -1 |
| G: -5311.25950 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.75690 HOMO: -6.69400 LUMO: -0.05442 factor:1 | 1 (-2.13171) | -1 | -1 |
| G: -5311.25950 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.96763 HOMO: -6.36202 LUMO: 0.09796 factor:1 | 1 (-2.34244) | -1 | -1 |
| G: -5311.25950 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.71554 HOMO: -6.54978 LUMO: 0.15510 factor:1 | 1 (-2.09035) | -1 | -1 |
| G: -5311.25950 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.29466 HOMO: -6.77836 LUMO: 0.25851 factor:1 | 1 (-1.66947) | -1 | -1 |
| G: -5311.25950 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.44297 HOMO: -5.70623 LUMO: 0.73471 factor:1 | 1 (-1.81778) | -1 | -1 |
| G: -5311.25950 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.58400 HOMO: -5.58378 LUMO: 0.89253 factor:1 | 1 (-1.95881) | -1 | -1 |
| G: -5311.25950 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.84418 HOMO: -5.68718 LUMO: 0.87893 factor:1 | 1 (-1.21899) | -1 | -1 |
| G: -5311.25950 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.94143 HOMO: -5.10486 LUMO: 1.11567 factor:1 | 1 (-1.31624) | -1 | -1 |
| G: -5311.25950 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.01006 HOMO: -4.59328 LUMO: 1.27621 factor:1 | 1 (-1.38487) | -1 | -1 |
| G: -5311.25950 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.90769 HOMO: -4.45450 LUMO: 1.82044 factor:1 | 1 (-1.28250) | -1 | -1 |
| G: -5311.25950 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.05496 HOMO: -4.64226 LUMO: 1.70615 factor:1 | 1 (-1.42977) | -1 | -1 |
| G: -5311.25950 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.99221 HOMO: -5.04227 LUMO: 1.04492 factor:1 | 1 (-1.36702) | -1 | -1 |
| G: -5311.25950 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.17472 HOMO: -4.85723 LUMO: 0.93607 factor:1 | 1 (-1.54953) | -1 | -1 |
| G: -5311.25950 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.13744 HOMO: -4.72934 LUMO: 1.00410 factor:1 | 1 (-1.51225) | -1 | -1 |
| G: -5311.25950 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.99251 HOMO: -4.56335 LUMO: 1.56738 factor:1 | 1 (-1.36732) | -1 | -1 |
| G: -5311.25950 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.84116 HOMO: -5.48854 LUMO: 0.33198 factor:1 | 1 (-1.21597) | -1 | -1 |
| G: -5311.25950 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.16936 HOMO: -4.97424 LUMO: 1.33608 factor:1 | 1 (-1.54416) | -1 | -1 |
| G: -5311.25950 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.78358 HOMO: -4.60145 LUMO: 1.74697 factor:1 | 1 (-1.15839) | -1 | -1 |
| G: -5311.25950 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.80780 HOMO: -5.60010 LUMO: 0.74831 factor:1 | 1 (-1.18261) | -1 | -1 |
| G: -5311.25950 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.70978 HOMO: -5.66541 LUMO: 0.66668 factor:1 | 1 (-1.08459) | -1 | -1 |
| G: -5311.25950 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.79713 HOMO: -6.50080 LUMO: 0.07075 factor:1 | 1 (-1.17194) | -1 | -1 |
| G: -5311.25950 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.78929 HOMO: -5.79603 LUMO: 0.22313 factor:1 | 1 (-1.16410) | -1 | -1 |
| G: -5311.25950 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.94217 HOMO: -4.68036 LUMO: 1.29798 factor:1 | 1 (-1.31698) | -1 | -1 |
| G: -5311.25950 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.12008 HOMO: -4.84363 LUMO: 1.34424 factor:1 | 1 (-1.49488) | -1 | -1 |
| G: -5311.25950 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.01882 HOMO: -4.62321 LUMO: 1.82861 factor:1 | 1 (-1.39363) | -1 | -1 |
| G: -5311.25950 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.95409 HOMO: -5.83684 LUMO: 0.82178 factor:1 | 1 (-1.32890) | -1 | -1 |
| G: -5311.25950 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.79112 HOMO: -5.27629 LUMO: 0.57960 factor:1 | 1 (-1.16593) | -1 | -1 |
| G: -5311.25950 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.77260 HOMO: -5.15928 LUMO: -2.96876 factor:1 | 1 (-2.14741) | -1 | -1 |
| G: -5311.25950 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.95446 HOMO: -5.08853 LUMO: 0.89253 factor:1 | 1 (-2.32927) | -1 | -1 |
| G: -5311.25950 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.84308 HOMO: -6.42461 LUMO: 0.04354 factor:1 | 1 (-2.21789) | -1 | -1 |
| G: -5311.25950 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.64814 HOMO: -6.42733 LUMO: -0.00544 factor:1 | 1 (-2.02295) | -1 | -1 |
| G: -5311.25950 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.96434 HOMO: -5.87494 LUMO: 0.69933 factor:1 | 1 (-2.33915) | -1 | -1 |
| G: -5311.25950 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.87887 HOMO: -5.07492 LUMO: 1.02587 factor:1 | 1 (-2.25367) | -1 | -1 |
| G: -5311.25950 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11578.05479 HOMO: -4.44362 LUMO: 1.99187 factor:1 | 1 (-2.42960) | -1 | -1 |
| G: -5311.25950 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.74382 HOMO: -5.82052 LUMO: 0.43810 factor:1 | 1 (-2.11862) | -1 | -1 |
| G: -5311.25950 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.70240 HOMO: -5.75793 LUMO: 0.76464 factor:1 | 1 (-2.07721) | -1 | -1 |
| G: -5311.25950 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11578.05517 HOMO: -5.09669 LUMO: 0.72382 factor:1 | 1 (-2.42998) | -1 | -1 |
| G: -5311.25950 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.78167 HOMO: -6.75387 LUMO: -2.02453 factor:1 | 1 (-2.15648) | -1 | -1 |
| G: -5311.25950 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.89421 HOMO: -5.02322 LUMO: 1.14832 factor:1 | 1 (-2.26902) | -1 | -1 |
| G: -5311.25950 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.70341 HOMO: -5.75521 LUMO: 0.73471 factor:1 | 1 (-2.07822) | -1 | -1 |
| G: -5311.25950 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.61546 HOMO: -5.89943 LUMO: 0.54967 factor:1 | 1 (-1.99027) | -1 | -1 |
| G: -5311.25950 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.47061 HOMO: -5.80147 LUMO: 0.72382 factor:1 | 1 (-1.84542) | -1 | -1 |
| G: -5311.25950 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.86670 HOMO: -6.16066 LUMO: 0.39457 factor:1 | 1 (-2.24151) | -1 | -1 |
| G: -5311.25950 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.66833 HOMO: -5.98650 LUMO: 0.76736 factor:1 | 1 (-2.04314) | -1 | -1 |
| G: -5311.25950 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.47921 HOMO: -4.74839 LUMO: 1.88847 factor:1 | 1 (-1.85402) | -1 | -1 |
| G: -5311.25950 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.68082 HOMO: -5.62459 LUMO: 0.26939 factor:1 | 1 (-2.05563) | -1 | -1 |
| G: -5311.25950 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.72773 HOMO: -4.88172 LUMO: 1.30070 factor:1 | 1 (-2.10254) | -1 | -1 |
| G: -5311.25950 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.64346 HOMO: -5.09397 LUMO: 0.98505 factor:1 | 1 (-2.01827) | -1 | -1 |
| G: -5311.25950 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: -0.28300 factor:1 | 1 (-2.19326) | -1 | -1 |
| G: -5311.25950 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.85870 HOMO: -5.04227 LUMO: 1.49935 factor:1 | 1 (-2.23351) | -1 | -1 |
| G: -5311.25950 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.66534 HOMO: -5.22731 LUMO: 0.88437 factor:1 | 1 (-2.04015) | -1 | -1 |
| G: -5311.25950 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.54071 HOMO: -4.95519 LUMO: 1.25717 factor:1 | 1 (-1.91552) | -1 | -1 |
| G: -5311.25950 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.36441 HOMO: -4.61233 LUMO: 1.27621 factor:1 | 1 (-1.73922) | -1 | -1 |
| G: -5311.25950 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.77329 HOMO: -4.70757 LUMO: 1.63813 factor:1 | 1 (-2.14809) | -1 | -1 |
| G: -5311.25950 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.58389 HOMO: -4.85179 LUMO: 1.11839 factor:1 | 1 (-1.95870) | -1 | -1 |
| G: -5311.25950 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.74156 HOMO: -4.97696 LUMO: 1.00138 factor:1 | 1 (-2.11637) | -1 | -1 |
| G: -5311.25950 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.42620 HOMO: -5.64636 LUMO: 0.81090 factor:1 | 1 (-1.80101) | -1 | -1 |
| G: -5311.25950 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.33679 HOMO: -4.37831 LUMO: 1.90208 factor:1 | 1 (-1.71160) | -1 | -1 |
| G: -5311.25950 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.57853 HOMO: -4.67764 LUMO: 1.54561 factor:1 | 1 (-1.95334) | -1 | -1 |
| G: -5311.25950 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.45037 HOMO: -5.87766 LUMO: 0.42994 factor:1 | 1 (-1.82518) | -1 | -1 |
| G: -5311.25950 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.77092 HOMO: -6.03821 LUMO: 0.32382 factor:1 | 1 (-2.14573) | -1 | -1 |
| G: -5311.25950 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.41891 HOMO: -5.99739 LUMO: 0.69389 factor:1 | 1 (-1.79372) | -1 | -1 |
| G: -5311.25950 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.15923 HOMO: -6.43821 LUMO: 0.15238 factor:1 | 1 (-1.53404) | -1 | -1 |
| G: -5311.25950 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.44599 HOMO: -6.63414 LUMO: -0.07347 factor:1 | 1 (-1.82080) | -1 | -1 |
| G: -5311.25950 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.71337 HOMO: -6.50080 LUMO: 0.10068 factor:1 | 1 (-2.08817) | -1 | -1 |
| G: -5311.25950 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.48161 HOMO: -6.49264 LUMO: 0.19592 factor:1 | 1 (-1.85642) | -1 | -1 |
| G: -5311.25950 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.53709 HOMO: -5.83956 LUMO: 0.12517 factor:1 | 1 (-1.91190) | -1 | -1 |
| G: -5311.25950 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.56223 HOMO: -6.50896 LUMO: 0.19048 factor:1 | 1 (-1.93704) | -1 | -1 |
| G: -5311.25950 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.74335 HOMO: -6.56611 LUMO: 0.04898 factor:1 | 1 (-2.11816) | -1 | -1 |
| G: -5311.25950 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.69473 HOMO: -6.68040 LUMO: -0.08436 factor:1 | 1 (-2.06953) | -1 | -1 |
| G: -5311.25950 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.60112 HOMO: -6.73754 LUMO: -0.08708 factor:1 | 1 (-1.97593) | -1 | -1 |
| G: -5311.25950 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.88172 HOMO: -6.80285 LUMO: -0.10612 factor:1 | 1 (-2.25653) | -1 | -1 |
| G: -5311.25950 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.58727 HOMO: -6.35658 LUMO: 0.02177 factor:1 | 1 (-1.96208) | -1 | -1 |
| G: -5311.25950 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.75617 HOMO: -5.74160 LUMO: 0.14694 factor:1 | 1 (-2.13098) | -1 | -1 |
| G: -5311.25950 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.61453 HOMO: -4.78376 LUMO: 0.92791 factor:1 | 1 (-1.98934) | -1 | -1 |
| G: -5311.25950 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.53644 HOMO: -5.90215 LUMO: 0.36463 factor:1 | 1 (-1.91125) | -1 | -1 |
| G: -5311.25950 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.42729 HOMO: -4.99329 LUMO: 0.85988 factor:1 | 1 (-1.80210) | -1 | -1 |
| G: -5311.25950 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.44610 HOMO: -4.93887 LUMO: 1.33608 factor:1 | 1 (-1.82090) | -1 | -1 |
| G: -5311.25950 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.71035 HOMO: -5.19193 LUMO: 0.50341 factor:1 | 1 (-2.08515) | -1 | -1 |
| G: -5311.25950 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.81843 HOMO: -6.64502 LUMO: -1.98643 factor:1 | 1 (-2.19324) | -1 | -1 |
| G: -5311.25950 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.60485 HOMO: -5.15384 LUMO: 0.94968 factor:1 | 1 (-1.97966) | -1 | -1 |
| G: -5311.25950 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.39369 HOMO: -6.31032 LUMO: 0.08436 factor:1 | 1 (-1.76850) | -1 | -1 |
| G: -5311.25950 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.43410 HOMO: -4.88716 LUMO: 0.82995 factor:1 | 1 (-1.80890) | -1 | -1 |
| G: -5311.25950 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.32702 HOMO: -5.57017 LUMO: 0.19320 factor:1 | 1 (-1.70183) | -1 | -1 |
| G: -5311.25950 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.18974 HOMO: -4.92254 LUMO: 0.93879 factor:1 | 1 (-1.56455) | -1 | -1 |
| G: -5311.25950 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.70643 HOMO: -4.77288 LUMO: 1.60003 factor:1 | 1 (-2.08124) | -1 | -1 |
| G: -5311.25950 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.48514 HOMO: -4.97696 LUMO: 0.89798 factor:1 | 1 (-1.85995) | -1 | -1 |
| G: -5311.25950 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.14612 HOMO: -5.00690 LUMO: 1.14288 factor:1 | 1 (-1.52093) | -1 | -1 |
| G: -5311.25950 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.21548 HOMO: -4.88444 LUMO: 1.48574 factor:1 | 1 (-1.59029) | -1 | -1 |
| G: -5311.25950 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.52841 HOMO: -5.03955 LUMO: 1.51023 factor:1 | 1 (-1.90322) | -1 | -1 |
| G: -5311.25950 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.30457 HOMO: -5.22459 LUMO: 0.99049 factor:1 | 1 (-1.67938) | -1 | -1 |
| G: -5311.25950 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.37135 HOMO: -5.29534 LUMO: 0.96056 factor:1 | 1 (-1.74615) | -1 | -1 |
| G: -5311.25950 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11578.10940 HOMO: -5.35520 LUMO: 0.68301 factor:1 | 1 (-2.48421) | -1 | -1 |
| G: -5311.25950 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11578.39055 HOMO: -5.27357 LUMO: 1.18642 factor:1 | 1 (-2.76536) | -1 | -1 |
| G: -5311.25950 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11578.98925 HOMO: -5.79875 LUMO: 0.61770 factor:1 | 1 (-3.36406) | -1 | -1 |
| G: -5311.25950 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.70591 HOMO: -7.64640 LUMO: -2.45175 factor:1 | 1 (-2.08072) | -1 | -1 |
| G: -5311.25950 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11578.13473 HOMO: -7.46953 LUMO: -1.29798 factor:1 | 1 (-2.50954) | 1 | 1 |
| G: -5311.25950 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.74743 HOMO: -7.95389 LUMO: -0.37280 factor:1 | 1 (-2.12224) | 1 | 1 |
| G: -5311.25950 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11578.17299 HOMO: -7.23279 LUMO: -1.19186 factor:1 | 1 (-2.54780) | 1 | 1 |
| G: -5311.25950 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.99476 HOMO: -7.14299 LUMO: -1.12927 factor:1 | 1 (-2.36957) | 1 | 1 |
| G: -5311.25950 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11578.38946 HOMO: -6.93074 LUMO: 0.31565 factor:1 | 1 (-2.76427) | -1 | -1 |
| G: -5311.25950 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11578.93761 HOMO: -6.63141 LUMO: 0.28028 factor:1 | 1 (-3.31241) | -1 | -1 |
| G: -5311.25950 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11578.19879 HOMO: -7.10489 LUMO: -1.07213 factor:1 | 1 (-2.57360) | 1 | 1 |
| G: -5311.25950 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11578.45123 HOMO: -7.00693 LUMO: -0.69389 factor:1 | 1 (-2.82604) | -1 | -1 |
| G: -5311.25950 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11579.10898 HOMO: -8.50356 LUMO: -1.79595 factor:1 | 1 (-3.48379) | -1 | -1 |
| G: -5311.25950 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11578.98863 HOMO: -7.79334 LUMO: -2.33746 factor:1 | 1 (-3.36344) | -1 | -1 |
| G: -5311.25950 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.81339 HOMO: -7.24367 LUMO: -0.85172 factor:1 | 1 (-2.18820) | 1 | 1 |
| G: -5311.25950 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.96306 HOMO: -7.94028 LUMO: -0.20136 factor:1 | 1 (-2.33787) | 1 | 1 |
| G: -5311.25950 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11578.29947 HOMO: -7.22462 LUMO: 0.84627 factor:1 | 1 (-2.67428) | 1 | 1 |
| G: -5311.25950 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11578.18761 HOMO: -6.54978 LUMO: 0.34831 factor:1 | 1 (-2.56241) | -1 | -1 |
| G: -5311.25950 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.91223 HOMO: -6.86815 LUMO: 0.32109 factor:1 | 1 (-2.28704) | -1 | -1 |
| G: -5311.25950 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.69005 HOMO: -7.17564 LUMO: -1.28438 factor:1 | 1 (-1.06486) | 1 | 1 |
| G: -5311.25950 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.85564 HOMO: -7.03142 LUMO: -1.12655 factor:1 | 1 (-1.23044) | -1 | -1 |
| G: -5311.25950 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.10307 HOMO: -7.39878 LUMO: 0.15783 factor:1 | 1 (-1.47788) | 1 | 1 |
| G: -5311.25950 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.79169 HOMO: -7.25728 LUMO: 0.42178 factor:1 | 1 (-1.16650) | 1 | 1 |
| G: -5311.25950 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.60589 HOMO: -6.86543 LUMO: 0.93879 factor:1 | 1 (-0.98070) | -1 | -1 |
| G: -5311.25950 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.64028 HOMO: -7.09673 LUMO: -0.69661 factor:1 | 1 (-1.01509) | 1 | 1 |
| G: -5311.25950 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.65004 HOMO: -7.74708 LUMO: 0.01088 factor:1 | 1 (-2.02485) | 1 | 1 |
| G: -5311.25950 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11578.51580 HOMO: -6.80557 LUMO: 0.46531 factor:1 | 1 (-2.89061) | -1 | -1 |
| G: -5311.25950 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.97723 HOMO: -7.29265 LUMO: 1.31975 factor:1 | 1 (-2.35204) | 1 | 1 |
| G: -5311.25950 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.83108 HOMO: -6.93618 LUMO: 0.29388 factor:1 | 1 (-2.20589) | -1 | -1 |
| G: -5311.25950 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.58085 HOMO: -6.53073 LUMO: 0.71022 factor:1 | 1 (-1.95566) | -1 | -1 |
| G: -5311.25950 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.70308 HOMO: -6.41917 LUMO: -1.24084 factor:1 | 1 (-2.07789) | -1 | -1 |
| G: -5311.25950 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.59279 HOMO: -6.67495 LUMO: -1.09118 factor:1 | 1 (-1.96760) | -1 | -1 |
| G: -5311.25950 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.80050 HOMO: -6.97156 LUMO: -0.53606 factor:1 | 1 (-2.17531) | -1 | -1 |
| G: -5311.25950 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.65772 HOMO: -6.85183 LUMO: -0.45715 factor:1 | 1 (-2.03253) | -1 | -1 |
| G: -5311.25950 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.96877 HOMO: -7.12666 LUMO: -0.67484 factor:1 | 1 (-2.34358) | 1 | 1 |
| G: -5311.25950 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.76395 HOMO: -7.49946 LUMO: -0.14694 factor:1 | 1 (-2.13876) | 1 | 1 |
| G: -5311.25950 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11578.12815 HOMO: -7.44231 LUMO: 0.58232 factor:1 | 1 (-2.50296) | 1 | 1 |
| G: -5311.25950 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.97669 HOMO: -7.36340 LUMO: -0.68301 factor:1 | 1 (-2.35150) | 1 | 1 |
| G: -5311.25950 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11578.22407 HOMO: -6.13073 LUMO: -0.54967 factor:1 | 1 (-2.59888) | -1 | -1 |
| G: -5311.25950 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11578.80087 HOMO: -7.81511 LUMO: -0.06531 factor:1 | 1 (-3.17568) | 1 | 1 |
| G: -5311.25950 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11578.38970 HOMO: -7.26816 LUMO: -1.02587 factor:1 | 1 (-2.76451) | 1 | 1 |
| G: -5311.25950 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11578.15218 HOMO: -7.98110 LUMO: -0.17960 factor:1 | 1 (-2.52699) | 1 | 1 |
| G: -5311.25950 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.71168 HOMO: -7.44776 LUMO: -1.00954 factor:1 | 1 (-2.08649) | 1 | 1 |
| G: -5311.25950 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.95879 HOMO: -7.47769 LUMO: -1.02859 factor:1 | 1 (-2.33359) | 1 | 1 |
| G: -5311.25950 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.95217 HOMO: -6.75659 LUMO: 0.39457 factor:1 | 1 (-2.32698) | -1 | -1 |
| G: -5311.25950 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.82006 HOMO: -6.71849 LUMO: 0.36735 factor:1 | 1 (-2.19487) | -1 | -1 |
| G: -5311.25950 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.56789 HOMO: -7.64096 LUMO: -1.43948 factor:1 | 1 (-1.94270) | 1 | 1 |
| G: -5311.25950 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.91496 HOMO: -7.83144 LUMO: -1.36601 factor:1 | 1 (-1.28977) | 1 | 1 |
| G: -5311.25950 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.82407 HOMO: -7.19469 LUMO: 0.35103 factor:1 | 1 (-1.19888) | 1 | 1 |
| G: -5311.25950 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.93324 HOMO: -7.03414 LUMO: 0.20409 factor:1 | 1 (-1.30805) | -1 | -1 |
| G: -5311.25950 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.17480 HOMO: -7.22734 LUMO: 0.31293 factor:1 | 1 (-1.54961) | 1 | 1 |
| G: -5311.25950 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.12565 HOMO: -6.93618 LUMO: 0.56055 factor:1 | 1 (-1.50046) | -1 | -1 |
| G: -5311.25950 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.96225 HOMO: -6.94707 LUMO: -0.88709 factor:1 | 1 (-1.33706) | -1 | -1 |
| G: -5311.25950 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.93771 HOMO: -6.86543 LUMO: -0.83267 factor:1 | 1 (-1.31251) | -1 | -1 |
| G: -5311.25950 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.74475 HOMO: -6.82189 LUMO: -1.15376 factor:1 | 1 (-1.11956) | -1 | -1 |
| G: -5311.25950 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.76276 HOMO: -6.65046 LUMO: -0.46531 factor:1 | 1 (-1.13757) | -1 | -1 |
| G: -5311.25950 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.68878 HOMO: -6.52529 LUMO: 0.20953 factor:1 | 1 (-1.06358) | -1 | -1 |
| G: -5311.25950 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.82366 HOMO: -6.80557 LUMO: 0.44355 factor:1 | 1 (-1.19847) | -1 | -1 |
| G: -5311.25950 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.95049 HOMO: -6.93074 LUMO: -0.81634 factor:1 | 1 (-1.32530) | -1 | -1 |
| G: -5311.25950 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.92440 HOMO: -7.43143 LUMO: -0.45987 factor:1 | 1 (-1.29921) | 1 | 1 |
| G: -5311.25950 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.05412 HOMO: -7.07224 LUMO: -0.68028 factor:1 | 1 (-1.42892) | 1 | 1 |
| G: -5311.25950 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.09031 HOMO: -6.68040 LUMO: -0.71566 factor:1 | 1 (-1.46512) | -1 | -1 |
| G: -5311.25950 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.87694 HOMO: -6.26406 LUMO: -1.09934 factor:1 | 1 (-1.25175) | -1 | -1 |
| G: -5311.25950 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.82834 HOMO: -5.94569 LUMO: -0.72110 factor:1 | 1 (-1.20315) | -1 | -1 |
| G: -5311.25950 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.66026 HOMO: -6.12256 LUMO: -0.42178 factor:1 | 1 (-1.03507) | -1 | -1 |
| G: -5311.25950 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.80815 HOMO: -6.09807 LUMO: 0.11429 factor:1 | 1 (-1.18296) | -1 | -1 |
| G: -5311.25950 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.68761 HOMO: -7.35252 LUMO: -0.55783 factor:1 | 1 (-1.06241) | 1 | 1 |
| G: -5311.25950 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.85621 HOMO: -7.57837 LUMO: -0.76736 factor:1 | 1 (-1.23102) | 1 | 1 |
| G: -5311.25950 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.69539 HOMO: -6.16066 LUMO: 0.01905 factor:1 | 1 (-1.07020) | -1 | -1 |
| G: -5311.25950 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.11999 HOMO: -6.13345 LUMO: -0.41906 factor:1 | 1 (-1.49480) | -1 | -1 |
| G: -5311.25950 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.89506 HOMO: -6.10351 LUMO: -0.33742 factor:1 | 1 (-1.26987) | -1 | -1 |
| G: -5311.25950 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.90440 HOMO: -7.24639 LUMO: -0.51702 factor:1 | 1 (-1.27921) | 1 | 1 |
| G: -5311.25950 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.75476 HOMO: -6.98244 LUMO: -1.82044 factor:1 | 1 (-1.12957) | -1 | -1 |
| G: -5311.25950 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.67280 HOMO: -6.37563 LUMO: -1.67622 factor:1 | 1 (-1.04761) | -1 | -1 |
| G: -5311.25950 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.55190 HOMO: -5.79058 LUMO: -2.55243 factor:1 | 1 (-0.92671) | -1 | -1 |
| G: -5311.25950 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.70110 HOMO: -6.34025 LUMO: -0.27483 factor:1 | 1 (-1.07591) | -1 | -1 |
| G: -5311.25950 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.94277 HOMO: -6.05453 LUMO: -0.51157 factor:1 | 1 (-1.31758) | -1 | -1 |
| G: -5311.25950 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11578.14483 HOMO: -7.53755 LUMO: -0.38912 factor:1 | 1 (-2.51964) | 1 | 1 |
| G: -5311.25950 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11579.07984 HOMO: -7.00421 LUMO: -0.50885 factor:1 | 1 (-3.45465) | -1 | -1 |
| G: -5311.25950 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11578.29335 HOMO: -7.52123 LUMO: -0.37552 factor:1 | 1 (-2.66816) | 1 | 1 |
| G: -5311.25950 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11578.20937 HOMO: -6.70489 LUMO: -1.04764 factor:1 | 1 (-2.58418) | -1 | -1 |
| G: -5311.25950 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.98635 HOMO: -7.06408 LUMO: -1.16737 factor:1 | 1 (-2.36116) | 1 | 1 |
| G: -5311.25950 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.75493 HOMO: -6.71849 LUMO: -1.02315 factor:1 | 1 (-1.12974) | -1 | -1 |
| G: -5311.25950 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.73351 HOMO: -6.16610 LUMO: -0.50885 factor:1 | 1 (-1.10832) | -1 | -1 |
| G: -5311.25950 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.96571 HOMO: -6.48447 LUMO: 0.07619 factor:1 | 1 (-1.34051) | -1 | -1 |
| G: -5311.25950 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.84187 HOMO: -7.06135 LUMO: 0.09796 factor:1 | 1 (-1.21668) | 1 | 1 |
| G: -5311.25950 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.59903 HOMO: -6.47359 LUMO: 0.22585 factor:1 | 1 (-0.97384) | -1 | -1 |
| G: -5311.25950 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.50972 HOMO: -6.10896 LUMO: -0.62314 factor:1 | 1 (-0.88453) | -1 | -1 |
| G: -5311.25950 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.69416 HOMO: -6.88176 LUMO: -0.96600 factor:1 | 1 (-1.06897) | -1 | -1 |
| G: -5311.25950 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.87185 HOMO: -6.67495 LUMO: 0.21769 factor:1 | 1 (-1.24666) | -1 | -1 |
| G: -5311.25950 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.73758 HOMO: -6.84911 LUMO: 0.38368 factor:1 | 1 (-2.11239) | -1 | -1 |
| G: -5311.25950 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11578.44568 HOMO: -6.83550 LUMO: 1.29798 factor:1 | 1 (-2.82049) | -1 | -1 |
| G: -5311.25950 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.76953 HOMO: -6.67495 LUMO: 1.46941 factor:1 | 1 (-2.14434) | -1 | -1 |
| G: -5311.25950 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.97966 HOMO: -6.81917 LUMO: 1.30887 factor:1 | 1 (-2.35447) | -1 | -1 |
| G: -5311.25950 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.87266 HOMO: -6.56611 LUMO: 0.66396 factor:1 | 1 (-2.24747) | -1 | -1 |
| G: -5311.25950 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.59456 HOMO: -6.76203 LUMO: 0.60137 factor:1 | 1 (-1.96937) | -1 | -1 |
| G: -5311.25950 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.75707 HOMO: -6.55794 LUMO: 0.34286 factor:1 | 1 (-2.13188) | -1 | -1 |
| G: -5311.25950 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.92602 HOMO: -6.83550 LUMO: 0.35919 factor:1 | 1 (-2.30083) | -1 | -1 |
| G: -5311.25950 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.78575 HOMO: -7.17836 LUMO: 0.63130 factor:1 | 1 (-2.16056) | 1 | 1 |
| G: -5311.25950 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.54844 HOMO: -6.29944 LUMO: -0.69389 factor:1 | 1 (-1.92325) | -1 | -1 |
| G: -5311.25950 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11578.10545 HOMO: -7.06680 LUMO: -0.95784 factor:1 | 1 (-2.48026) | 1 | 1 |
| G: -5311.25950 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.93704 HOMO: -6.84638 LUMO: -0.87076 factor:1 | 1 (-2.31185) | -1 | -1 |
| G: -5311.25950 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11578.16984 HOMO: -6.96339 LUMO: -1.05308 factor:1 | 1 (-2.54465) | -1 | -1 |
| G: -5311.25950 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.91927 HOMO: -6.75387 LUMO: -1.04220 factor:1 | 1 (-2.29408) | -1 | -1 |
| G: -5311.25950 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11578.07949 HOMO: -6.71849 LUMO: -0.84355 factor:1 | 1 (-2.45430) | -1 | -1 |
| G: -5311.25950 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.76567 HOMO: -7.16748 LUMO: 0.51702 factor:1 | 1 (-1.14048) | 1 | 1 |
| G: -5311.25950 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.54853 HOMO: -6.92530 LUMO: 0.71566 factor:1 | 1 (-0.92334) | -1 | -1 |
| G: -5311.25950 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.85596 HOMO: -7.11034 LUMO: 0.01905 factor:1 | 1 (-1.23077) | 1 | -1 |
| G: -5311.25950 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.59808 HOMO: -6.79468 LUMO: 0.77008 factor:1 | 1 (-0.97289) | -1 | -1 |
| G: -5311.25950 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.81115 HOMO: -6.52801 LUMO: 0.98233 factor:1 | 1 (-1.18595) | -1 | -1 |
| G: -5311.25950 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.78461 HOMO: -6.76475 LUMO: 0.53334 factor:1 | 1 (-1.15942) | -1 | -1 |
| G: -5311.25950 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.56692 HOMO: -5.29261 LUMO: 0.57416 factor:1 | 1 (-0.94173) | -1 | -1 |
| G: -5311.25950 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.54436 HOMO: -6.57971 LUMO: 0.12789 factor:1 | 1 (-0.91917) | -1 | -1 |
| G: -5311.25950 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.34899 HOMO: -6.99333 LUMO: 0.51430 factor:1 | 1 (-0.72380) | -1 | -1 |
| G: -5311.25950 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.72344 HOMO: -6.41917 LUMO: 0.19048 factor:1 | 1 (-1.09825) | -1 | -1 |
| G: -5311.25950 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.74235 HOMO: -6.16066 LUMO: 1.77146 factor:1 | 1 (-2.11715) | -1 | -1 |
| G: -5311.25950 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.55516 HOMO: -6.90353 LUMO: 1.65717 factor:1 | 1 (-1.92997) | -1 | -1 |
| G: -5311.25950 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11578.59292 HOMO: -5.94569 LUMO: 1.29526 factor:1 | 1 (-2.96773) | -1 | -1 |
| G: -5311.25950 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.58553 HOMO: -6.60420 LUMO: 1.33880 factor:1 | 1 (-1.96034) | -1 | -1 |
| G: -5311.25950 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.82621 HOMO: -6.23957 LUMO: 0.09524 factor:1 | 1 (-2.20102) | -1 | -1 |
| G: -5311.25950 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.78539 HOMO: -6.80013 LUMO: 1.34696 factor:1 | 1 (-2.16020) | -1 | -1 |
| G: -5311.25950 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.81100 HOMO: -7.53483 LUMO: -1.52384 factor:1 | 1 (-2.18581) | -1 | -1 |
| G: -5311.25950 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.61336 HOMO: -7.62463 LUMO: -1.65717 factor:1 | 1 (-1.98817) | -1 | -1 |
| G: -5311.25950 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.80537 HOMO: -7.62463 LUMO: -1.61364 factor:1 | 1 (-2.18018) | -1 | -1 |
| G: -5311.25950 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.02780 HOMO: -8.04096 LUMO: -1.66806 factor:1 | 1 (-1.40261) | -1 | -1 |
| G: -5311.25950 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.89789 HOMO: -7.18381 LUMO: -1.17553 factor:1 | 1 (-1.27270) | 1 | 1 |
| G: -5311.25950 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.94946 HOMO: -7.69538 LUMO: -1.36601 factor:1 | 1 (-1.32427) | 1 | 1 |
| G: -5311.25950 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.06759 HOMO: -7.95117 LUMO: -1.48302 factor:1 | 1 (-1.44239) | -1 | -1 |
| G: -5311.25950 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.90641 HOMO: -6.98516 LUMO: 0.35919 factor:1 | 1 (-1.28122) | -1 | -1 |
| G: -5311.25950 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.71041 HOMO: -7.91579 LUMO: -0.32109 factor:1 | 1 (-1.08522) | 1 | 1 |
| G: -5311.25950 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.81270 HOMO: -6.75659 LUMO: -0.03537 factor:1 | 1 (-1.18750) | -1 | -1 |
| G: -5311.25950 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.96054 HOMO: -7.78518 LUMO: -2.36467 factor:1 | 1 (-1.33534) | -1 | -1 |
| G: -5311.25950 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.21268 HOMO: -7.96477 LUMO: -2.75651 factor:1 | 1 (-1.58749) | -1 | -1 |
| G: -5311.25950 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.08187 HOMO: -7.60286 LUMO: -2.35106 factor:1 | 1 (-1.45668) | -1 | -1 |
| G: -5311.25950 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.20574 HOMO: -7.38245 LUMO: -1.21635 factor:1 | 1 (-1.58055) | 1 | 1 |
| G: -5311.25950 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.07199 HOMO: -7.91579 LUMO: -1.50479 factor:1 | 1 (-1.44680) | -1 | -1 |
| G: -5311.25950 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.04816 HOMO: -8.07362 LUMO: -0.28028 factor:1 | 1 (-1.42297) | 1 | 1 |
| G: -5311.25950 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.85226 HOMO: -7.38245 LUMO: -1.15921 factor:1 | 1 (-1.22707) | 1 | 1 |
| G: -5311.25950 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.98435 HOMO: -7.18653 LUMO: -0.94968 factor:1 | 1 (-1.35915) | 1 | 1 |
| G: -5311.25950 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.01730 HOMO: -6.88448 LUMO: 0.38096 factor:1 | 1 (-1.39211) | -1 | -1 |
| G: -5311.25950 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.18955 HOMO: -6.97972 LUMO: 0.43266 factor:1 | 1 (-1.56436) | -1 | -1 |
| G: -5311.25950 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.97814 HOMO: -6.88992 LUMO: -0.43538 factor:1 | 1 (-1.35295) | -1 | -1 |
| G: -5311.25950 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.21940 HOMO: -7.97021 LUMO: -0.17143 factor:1 | 1 (-1.59421) | 1 | 1 |
| G: -5311.25950 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.05120 HOMO: -6.92530 LUMO: 0.77280 factor:1 | 1 (-1.42601) | -1 | -1 |
| G: -5311.25950 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.80480 HOMO: -7.89674 LUMO: -0.09796 factor:1 | 1 (-1.17961) | 1 | 1 |
| G: -5311.25950 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.98315 HOMO: -7.02870 LUMO: 0.88709 factor:1 | 1 (-1.35796) | -1 | -1 |
| G: -5311.25950 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.86979 HOMO: -6.78380 LUMO: 0.22041 factor:1 | 1 (-1.24459) | -1 | -1 |
| G: -5311.25950 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.76970 HOMO: -7.24911 LUMO: -0.82178 factor:1 | 1 (-1.14451) | 1 | 1 |
| G: -5311.25950 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.98927 HOMO: -6.77019 LUMO: 0.52790 factor:1 | 1 (-1.36408) | -1 | -1 |
| G: -5311.25950 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.84516 HOMO: -8.56070 LUMO: -1.83405 factor:1 | 1 (-1.21997) | -1 | -1 |
| G: -5311.25950 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.12816 HOMO: -7.74164 LUMO: -2.36195 factor:1 | 1 (-1.50297) | -1 | -1 |
| G: -5311.25950 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.92805 HOMO: -7.39878 LUMO: -2.41637 factor:1 | 1 (-1.30285) | -1 | -1 |
| G: -5311.25950 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.12729 HOMO: -7.61647 LUMO: -2.34018 factor:1 | 1 (-1.50210) | -1 | -1 |
| G: -5311.25950 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.93028 HOMO: -6.93346 LUMO: -0.57688 factor:1 | 1 (-1.30509) | -1 | -1 |
| G: -5311.25950 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.77710 HOMO: -6.85183 LUMO: -1.00410 factor:1 | 1 (-1.15191) | -1 | -1 |
| G: -5311.25950 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.84151 HOMO: -7.18925 LUMO: -1.12655 factor:1 | 1 (-1.21632) | 1 | 1 |
| G: -5311.25950 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.59060 HOMO: -6.85183 LUMO: -1.60275 factor:1 | 1 (-0.96541) | -1 | -1 |
| G: -5311.25950 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.63027 HOMO: -7.51578 LUMO: 0.12517 factor:1 | 1 (-1.00508) | 1 | 1 |
| G: -5311.25950 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.60276 HOMO: -7.36068 LUMO: 0.05714 factor:1 | 1 (-0.97757) | 1 | 1 |
| G: -5311.25950 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.47770 HOMO: -7.49674 LUMO: 0.18776 factor:1 | 1 (-0.85251) | 1 | 1 |
| G: -5311.25950 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.97346 HOMO: -7.09401 LUMO: -1.24900 factor:1 | 1 (-1.34827) | 1 | 1 |
| G: -5311.25950 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.07588 HOMO: -7.22462 LUMO: -1.61364 factor:1 | 1 (-1.45069) | -1 | -1 |
| G: -5311.25950 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.02892 HOMO: -7.74436 LUMO: -0.18776 factor:1 | 1 (-1.40373) | 1 | 1 |
| G: -5311.25950 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.90965 HOMO: -7.35252 LUMO: 0.75376 factor:1 | 1 (-1.28446) | 1 | 1 |
| G: -5311.25950 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.13540 HOMO: -7.75252 LUMO: 0.00816 factor:1 | 1 (-1.51020) | 1 | 1 |
| G: -5311.25950 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.24680 HOMO: -7.06680 LUMO: 0.24490 factor:1 | 1 (-1.62161) | 1 | 1 |
| G: -5311.25950 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.13428 HOMO: -7.49129 LUMO: 0.14150 factor:1 | 1 (-1.50909) | 1 | 1 |
| G: -5311.25950 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.15844 HOMO: -6.90625 LUMO: -1.11295 factor:1 | 1 (-1.53325) | -1 | -1 |
| G: -5311.25950 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.02046 HOMO: -6.78380 LUMO: -0.93063 factor:1 | 1 (-1.39526) | -1 | -1 |
| G: -5311.25950 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.83944 HOMO: -7.79878 LUMO: 0.30477 factor:1 | 1 (-1.21425) | 1 | 1 |
| G: -5311.25950 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.77604 HOMO: -7.87498 LUMO: 0.61770 factor:1 | 1 (-1.15085) | 1 | 1 |
| G: -5311.25950 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.79210 HOMO: -7.23823 LUMO: 0.30205 factor:1 | 1 (-1.16691) | 1 | 1 |
| G: -5311.25950 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.98617 HOMO: -7.67633 LUMO: 0.13061 factor:1 | 1 (-1.36098) | 1 | 1 |
| G: -5311.25950 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.66085 HOMO: -7.79606 LUMO: 0.34558 factor:1 | 1 (-2.03566) | 1 | 1 |
| G: -5311.25950 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.42819 HOMO: -6.66135 LUMO: -2.60141 factor:1 | 1 (-1.80300) | -1 | -1 |
| G: -5311.25950 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.75987 HOMO: -7.03142 LUMO: 0.50885 factor:1 | 1 (-2.13468) | -1 | -1 |
| G: -5311.25950 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.91451 HOMO: -7.05591 LUMO: -0.06531 factor:1 | 1 (-2.28932) | -1 | -1 |
| G: -5311.25950 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.72196 HOMO: -7.45592 LUMO: -1.39594 factor:1 | 1 (-2.09677) | 1 | 1 |
| G: -5311.25950 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.96485 HOMO: -7.22462 LUMO: -1.10478 factor:1 | 1 (-2.33966) | 1 | 1 |
| G: -5311.25950 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.49037 HOMO: -8.14709 LUMO: -0.55783 factor:1 | 1 (-1.86518) | 1 | 1 |
| G: -5311.25950 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.46819 HOMO: -7.22190 LUMO: -1.14560 factor:1 | 1 (-1.84300) | 1 | 1 |
| G: -5311.25950 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.34155 HOMO: -7.28721 LUMO: -1.14016 factor:1 | 1 (-1.71636) | 1 | 1 |
| G: -5311.25950 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.64501 HOMO: -6.97156 LUMO: 0.51702 factor:1 | 1 (-2.01982) | -1 | -1 |
| G: -5311.25950 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.70632 HOMO: -7.37156 LUMO: 0.29388 factor:1 | 1 (-2.08113) | 1 | -1 |
| G: -5311.25950 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.79822 HOMO: -7.66273 LUMO: -1.59731 factor:1 | 1 (-1.17303) | -1 | -1 |
| G: -5311.25950 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.84396 HOMO: -7.50490 LUMO: -1.49935 factor:1 | 1 (-1.21877) | -1 | -1 |
| G: -5311.25950 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.08105 HOMO: -7.61102 LUMO: -1.45581 factor:1 | 1 (-1.45586) | 1 | 1 |
| G: -5311.25950 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.68439 HOMO: -7.58653 LUMO: -1.61091 factor:1 | 1 (-1.05920) | -1 | -1 |
| G: -5311.25950 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.87164 HOMO: -7.36068 LUMO: -1.14560 factor:1 | 1 (-1.24644) | 1 | 1 |
| G: -5311.25950 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.73591 HOMO: -6.96339 LUMO: 0.26939 factor:1 | 1 (-1.11071) | -1 | -1 |
| G: -5311.25950 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.89139 HOMO: -6.53617 LUMO: 0.22313 factor:1 | 1 (-1.26620) | -1 | -1 |
| G: -5311.25950 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.15583 HOMO: -7.33619 LUMO: -1.02587 factor:1 | 1 (-1.53064) | 1 | 1 |
| G: -5311.25950 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.85346 HOMO: -6.87904 LUMO: 0.33742 factor:1 | 1 (-1.22827) | -1 | -1 |
| G: -5311.25950 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.84862 HOMO: -6.88448 LUMO: 0.58777 factor:1 | 1 (-1.22342) | -1 | -1 |
| G: -5311.25950 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.71857 HOMO: -6.55522 LUMO: -1.51295 factor:1 | 1 (-1.09338) | -1 | -1 |
| G: -5311.25950 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.41503 HOMO: -7.43415 LUMO: 0.10612 factor:1 | 1 (-0.78984) | 1 | 1 |
| G: -5311.25950 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.74089 HOMO: -7.54300 LUMO: -0.02449 factor:1 | 1 (-1.11569) | 1 | 1 |
| G: -5311.25950 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.96562 HOMO: -7.42054 LUMO: 0.28028 factor:1 | 1 (-1.34043) | 1 | 1 |
| G: -5311.25950 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.63555 HOMO: -6.98244 LUMO: -0.95784 factor:1 | 1 (-1.01036) | -1 | -1 |
| G: -5311.25950 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.75743 HOMO: -6.96884 LUMO: -1.12383 factor:1 | 1 (-1.13224) | -1 | -1 |
| G: -5311.25950 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.54842 HOMO: -6.80829 LUMO: -0.98233 factor:1 | 1 (-0.92323) | -1 | -1 |
| G: -5311.25950 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.11017 HOMO: -7.60830 LUMO: 0.58504 factor:1 | 1 (-1.48498) | 1 | 1 |
| G: -5311.25950 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.75640 HOMO: -7.52123 LUMO: 0.08163 factor:1 | 1 (-1.13120) | 1 | 1 |
| G: -5311.25950 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.62377 HOMO: -7.59742 LUMO: 0.00272 factor:1 | 1 (-0.99858) | 1 | 1 |
| G: -5311.25950 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.77509 HOMO: -6.99333 LUMO: -1.33880 factor:1 | 1 (-1.14990) | -1 | -1 |
| G: -5311.25950 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.97354 HOMO: -6.63958 LUMO: -1.39322 factor:1 | 1 (-1.34835) | -1 | -1 |
| G: -5311.25950 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.72023 HOMO: -7.86137 LUMO: 0.01633 factor:1 | 1 (-1.09504) | 1 | 1 |
| G: -5311.25950 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.50423 HOMO: -7.29537 LUMO: 0.14694 factor:1 | 1 (-0.87904) | 1 | 1 |
| G: -5311.25950 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.76668 HOMO: -6.95523 LUMO: 0.48708 factor:1 | 1 (-1.14149) | -1 | -1 |
| G: -5311.25950 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.78328 HOMO: -7.10217 LUMO: -1.10478 factor:1 | 1 (-1.15809) | 1 | 1 |
| G: -5311.25950 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.83596 HOMO: -6.88176 LUMO: -0.96328 factor:1 | 1 (-1.21077) | -1 | -1 |
| G: -5311.25950 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.87879 HOMO: -7.89130 LUMO: -0.13334 factor:1 | 1 (-1.25360) | 1 | 1 |
| G: -5311.25950 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.06726 HOMO: -7.75252 LUMO: 0.25579 factor:1 | 1 (-1.44207) | 1 | 1 |
| G: -5311.25950 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.90992 HOMO: -6.87632 LUMO: -0.93063 factor:1 | 1 (-1.28473) | -1 | -1 |
| G: -5311.25950 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.82649 HOMO: -6.78108 LUMO: -0.86804 factor:1 | 1 (-1.20130) | -1 | -1 |
| G: -5311.25950 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.70554 HOMO: -5.98106 LUMO: 0.10340 factor:1 | 1 (-1.08035) | -1 | -1 |
| G: -5311.25950 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.90200 HOMO: -6.40284 LUMO: -0.87349 factor:1 | 1 (-1.27681) | -1 | -1 |
| G: -5311.25950 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.74407 HOMO: -6.77019 LUMO: -1.20819 factor:1 | 1 (-1.11888) | -1 | -1 |
| G: -5311.25950 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.78516 HOMO: -6.90081 LUMO: -1.00682 factor:1 | 1 (-1.15997) | -1 | -1 |
| G: -5311.25950 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.54807 HOMO: -6.59060 LUMO: -0.26667 factor:1 | 1 (-0.92287) | -1 | -1 |
| G: -5311.25950 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.60782 HOMO: -6.50896 LUMO: -0.48708 factor:1 | 1 (-0.98263) | -1 | -1 |
| G: -5311.25950 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.43008 HOMO: -6.20420 LUMO: -0.73471 factor:1 | 1 (-0.80489) | -1 | -1 |
| G: -5311.25950 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.74780 HOMO: -6.17154 LUMO: -0.68573 factor:1 | 1 (-1.12261) | -1 | -1 |
| G: -5311.25950 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.09861 HOMO: -6.21236 LUMO: 0.09796 factor:1 | 1 (-1.47341) | -1 | -1 |
| G: -5311.25950 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.96581 HOMO: -6.38379 LUMO: 0.58232 factor:1 | 1 (-1.34062) | -1 | -1 |
| G: -5311.25950 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.06669 HOMO: -7.42871 LUMO: 0.40273 factor:1 | 1 (-1.44150) | 1 | 1 |
| G: -5311.25950 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.95052 HOMO: -6.54978 LUMO: 0.26395 factor:1 | 1 (-1.32533) | -1 | -1 |
| G: -5311.25950 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.89381 HOMO: -7.14027 LUMO: 0.14150 factor:1 | 1 (-1.26862) | 1 | 1 |
| G: -5311.25950 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.75468 HOMO: -7.25456 LUMO: -0.15783 factor:1 | 1 (-1.12949) | 1 | 1 |
| G: -5311.25950 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.78323 HOMO: -6.90897 LUMO: 0.63403 factor:1 | 1 (-1.15803) | -1 | -1 |
| G: -5311.25950 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.71925 HOMO: -6.49264 LUMO: 0.71022 factor:1 | 1 (-1.09406) | -1 | -1 |
| G: -5311.25950 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.99975 HOMO: -6.56067 LUMO: -1.03947 factor:1 | 1 (-1.37456) | -1 | -1 |
| G: -5311.25950 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.68366 HOMO: -6.79196 LUMO: -1.12655 factor:1 | 1 (-1.05847) | -1 | -1 |
| G: -5311.25950 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.91482 HOMO: -6.95251 LUMO: -1.09118 factor:1 | 1 (-1.28963) | -1 | -1 |
| G: -5311.25950 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.63188 HOMO: -7.47225 LUMO: -0.22041 factor:1 | 1 (-1.00669) | 1 | 1 |
| G: -5311.25950 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.78793 HOMO: -7.13483 LUMO: -0.98505 factor:1 | 1 (-1.16274) | 1 | 1 |
| G: -5311.25950 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.48265 HOMO: -6.99061 LUMO: -1.05852 factor:1 | 1 (-0.85746) | -1 | -1 |
| G: -5311.25950 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.77427 HOMO: -6.52257 LUMO: -1.11022 factor:1 | 1 (-1.14908) | -1 | -1 |
| G: -5311.25950 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.60766 HOMO: -6.75114 LUMO: -1.09934 factor:1 | 1 (-0.98247) | -1 | -1 |
| G: -5311.25950 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.65694 HOMO: -6.82189 LUMO: -0.89253 factor:1 | 1 (-1.03175) | -1 | -1 |
| G: -5311.25950 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.39843 HOMO: -6.83278 LUMO: -0.97961 factor:1 | 1 (-0.77324) | -1 | -1 |
| G: -5311.25950 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.97479 HOMO: -6.65318 LUMO: -0.84355 factor:1 | 1 (-1.34960) | -1 | -1 |
| G: -5311.25950 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.03743 HOMO: -6.75931 LUMO: -0.88437 factor:1 | 1 (-1.41224) | -1 | -1 |
| G: -5311.25950 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.13760 HOMO: -6.19059 LUMO: -0.45715 factor:1 | 1 (-1.51241) | -1 | -1 |
| G: -5311.25950 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.09050 HOMO: -7.09673 LUMO: -2.01908 factor:1 | 1 (-1.46531) | -1 | -1 |
| G: -5311.25950 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.11341 HOMO: -7.88042 LUMO: 0.38640 factor:1 | 1 (-1.48822) | 1 | 1 |
| G: -5311.25950 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.85264 HOMO: -7.83144 LUMO: 0.14422 factor:1 | 1 (-1.22745) | 1 | 1 |
| G: -5311.25950 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.86195 HOMO: -7.46408 LUMO: 0.44627 factor:1 | 1 (-1.23676) | 1 | 1 |
| G: -5311.25950 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.26843 HOMO: -7.12394 LUMO: -2.04902 factor:1 | 1 (-1.64324) | -1 | -1 |
| G: -5311.25950 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.09311 HOMO: -6.78380 LUMO: -1.11295 factor:1 | 1 (-1.46792) | -1 | -1 |
| G: -5311.25950 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.16642 HOMO: -7.12938 LUMO: -0.23674 factor:1 | 1 (-1.54123) | 1 | 1 |
| G: -5311.25950 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.03765 HOMO: -6.14705 LUMO: -0.20409 factor:1 | 1 (-1.41246) | -1 | -1 |
| G: -5311.25950 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.96701 HOMO: -6.50080 LUMO: -0.28300 factor:1 | 1 (-1.34182) | -1 | -1 |
| G: -5311.25950 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.95469 HOMO: -6.50352 LUMO: -0.62042 factor:1 | 1 (-1.32949) | -1 | -1 |
| G: -5311.25950 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.96048 HOMO: -6.46543 LUMO: -0.53879 factor:1 | 1 (-1.33529) | -1 | -1 |
| G: -5311.25950 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.07602 HOMO: -7.32803 LUMO: -0.52790 factor:1 | 1 (-1.45083) | 1 | 1 |
| G: -5311.25950 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.20103 HOMO: -5.94025 LUMO: -0.17687 factor:1 | 1 (-1.57584) | -1 | -1 |
| G: -5311.25950 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.24808 HOMO: -5.62187 LUMO: 0.05714 factor:1 | 1 (-1.62289) | -1 | -1 |
| G: -5311.25950 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.09031 HOMO: -7.03414 LUMO: -1.04492 factor:1 | 1 (-1.46512) | -1 | -1 |
| G: -5311.25950 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.04266 HOMO: -6.75387 LUMO: -2.02181 factor:1 | 1 (-1.41747) | -1 | -1 |
| G: -5311.25950 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.75539 HOMO: -6.55250 LUMO: -0.75648 factor:1 | 1 (-1.13020) | -1 | -1 |
| G: -5311.25950 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.75144 HOMO: -6.81101 LUMO: -1.02043 factor:1 | 1 (-1.12625) | -1 | -1 |
| G: -5311.25950 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.83623 HOMO: -6.69672 LUMO: -2.81910 factor:1 | 1 (-1.21104) | -1 | -1 |
| G: -5311.25950 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.10974 HOMO: -6.69128 LUMO: -2.58236 factor:1 | 1 (-1.48454) | -1 | -1 |
| G: -5311.25950 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.86965 HOMO: -6.73482 LUMO: -2.06807 factor:1 | 1 (-1.24446) | -1 | -1 |
| G: -5311.25950 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.16359 HOMO: -7.66545 LUMO: 0.17143 factor:1 | 1 (-1.53840) | 1 | 1 |
| G: -5311.25950 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.74208 HOMO: -6.87904 LUMO: -1.25172 factor:1 | 1 (-1.11689) | -1 | -1 |
| G: -5311.25950 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.93556 HOMO: -6.84366 LUMO: -0.19320 factor:1 | 1 (-1.31036) | -1 | -1 |
| G: -5311.25950 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.76067 HOMO: -6.97972 LUMO: -0.97961 factor:1 | 1 (-1.13548) | -1 | -1 |
| G: -5311.25950 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.54066 HOMO: -6.72121 LUMO: -0.70477 factor:1 | 1 (-0.91547) | -1 | -1 |
| G: -5311.25950 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.68371 HOMO: -7.18925 LUMO: 0.40001 factor:1 | 1 (-1.05852) | 1 | 1 |
| G: -5311.25950 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.86832 HOMO: -6.72121 LUMO: 0.19592 factor:1 | 1 (-1.24312) | -1 | -1 |
| G: -5311.25950 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.85022 HOMO: -6.85999 LUMO: -0.39457 factor:1 | 1 (-1.22503) | -1 | -1 |
| G: -5311.25950 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.12492 HOMO: -6.90625 LUMO: 0.05987 factor:1 | 1 (-1.49973) | -1 | -1 |
| G: -5311.25950 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.86192 HOMO: -7.00421 LUMO: 0.37552 factor:1 | 1 (-1.23673) | -1 | -1 |
| G: -5311.25950 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.96160 HOMO: -6.56883 LUMO: -0.97689 factor:1 | 1 (-1.33641) | -1 | -1 |
| G: -5311.25950 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.74148 HOMO: -6.66679 LUMO: 0.56055 factor:1 | 1 (-1.11629) | -1 | -1 |
| G: -5311.25950 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.05752 HOMO: -6.75931 LUMO: 0.32926 factor:1 | 1 (-1.43233) | -1 | -1 |
| G: -5311.25950 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.20187 HOMO: -6.53617 LUMO: -1.06397 factor:1 | 1 (-1.57668) | -1 | -1 |
| G: -5311.25950 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.82102 HOMO: -6.78108 LUMO: 0.42722 factor:1 | 1 (-1.19583) | -1 | -1 |
| G: -5311.25950 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.64412 HOMO: -7.05319 LUMO: 0.61498 factor:1 | 1 (-1.01893) | -1 | -1 |
| G: -5311.25950 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.94372 HOMO: -6.78380 LUMO: 1.49391 factor:1 | 1 (-1.31853) | -1 | -1 |
| G: -5311.25950 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.71166 HOMO: -7.21102 LUMO: 0.27211 factor:1 | 1 (-1.08647) | 1 | 1 |
| G: -5311.25950 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.63095 HOMO: -6.67223 LUMO: 0.81362 factor:1 | 1 (-1.00576) | -1 | -1 |
| G: -5311.25950 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.45688 HOMO: -6.69944 LUMO: 1.40683 factor:1 | 1 (-0.83169) | -1 | -1 |
| G: -5311.25950 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.96328 HOMO: -7.02598 LUMO: 1.46941 factor:1 | 1 (-1.33809) | -1 | -1 |
| G: -5311.25950 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.91428 HOMO: -5.85045 LUMO: -0.76736 factor:1 | 1 (-1.28908) | -1 | -1 |
| G: -5311.25950 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.16329 HOMO: -6.53890 LUMO: -0.50885 factor:1 | 1 (-1.53810) | -1 | -1 |
| G: -5311.25950 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.81452 HOMO: -6.42733 LUMO: -0.63947 factor:1 | 1 (-1.18933) | -1 | -1 |
| G: -5311.25950 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.68905 HOMO: -6.82189 LUMO: -0.85444 factor:1 | 1 (-1.06386) | -1 | -1 |
| G: -5311.25950 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.73563 HOMO: -6.97428 LUMO: -1.22179 factor:1 | 1 (-1.11044) | -1 | -1 |
| G: -5311.25950 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.96845 HOMO: -6.93346 LUMO: -1.09934 factor:1 | 1 (-1.34326) | -1 | -1 |
| G: -5311.25950 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.71142 HOMO: -7.17292 LUMO: -1.11839 factor:1 | 1 (-1.08622) | 1 | 1 |
| G: -5311.25950 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.72592 HOMO: -7.00965 LUMO: -1.23268 factor:1 | 1 (-1.10073) | -1 | -1 |
| G: -5311.25950 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.52129 HOMO: -6.73210 LUMO: -1.12383 factor:1 | 1 (-0.89610) | -1 | -1 |
| G: -5311.25950 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.59177 HOMO: -7.61375 LUMO: -0.11973 factor:1 | 1 (-0.96658) | 1 | 1 |
| G: -5311.25950 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.54140 HOMO: -7.42327 LUMO: 0.41906 factor:1 | 1 (-0.91621) | 1 | 1 |
| G: -5311.25950 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.32188 HOMO: -6.94162 LUMO: -1.01771 factor:1 | 1 (-0.69669) | -1 | -1 |
| G: -5311.25950 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.75631 HOMO: -6.82189 LUMO: -0.92791 factor:1 | 1 (-1.13112) | -1 | -1 |
| G: -5311.25950 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.63870 HOMO: -6.92258 LUMO: -1.73881 factor:1 | 1 (-2.01351) | -1 | -1 |
| G: -5311.25950 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.80153 HOMO: -6.50896 LUMO: -1.60819 factor:1 | 1 (-2.17634) | -1 | -1 |
| G: -5311.25950 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.67432 HOMO: -6.38379 LUMO: -2.18780 factor:1 | 1 (-2.04913) | -1 | -1 |
| G: -5311.25950 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.73644 HOMO: -6.48992 LUMO: -0.97417 factor:1 | 1 (-2.11125) | -1 | -1 |
| G: -5311.25950 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.96877 HOMO: -6.01644 LUMO: -0.04354 factor:1 | 1 (-2.34358) | -1 | -1 |
| G: -5311.25950 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.95876 HOMO: -6.70761 LUMO: -0.14422 factor:1 | 1 (-2.33357) | -1 | -1 |
| G: -5311.25950 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.90872 HOMO: -6.70216 LUMO: 0.14422 factor:1 | 1 (-2.28353) | -1 | -1 |
| G: -5311.25950 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.92774 HOMO: -7.07224 LUMO: -0.10885 factor:1 | 1 (-2.30255) | 1 | 1 |
| G: -5311.25950 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.65769 HOMO: -7.52667 LUMO: -0.74287 factor:1 | 1 (-2.03250) | 1 | 1 |
| G: -5311.25950 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.63043 HOMO: -6.48447 LUMO: -0.96056 factor:1 | 1 (-2.00523) | -1 | -1 |
| G: -5311.25950 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.45026 HOMO: -6.22597 LUMO: -0.41361 factor:1 | 1 (-1.82507) | -1 | -1 |
| G: -5311.25950 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.56498 HOMO: -6.12256 LUMO: -1.05852 factor:1 | 1 (-1.93979) | -1 | -1 |
| G: -5311.25950 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.49097 HOMO: -6.97428 LUMO: -0.60681 factor:1 | 1 (-1.86578) | -1 | -1 |
| G: -5311.25950 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.48065 HOMO: -6.78380 LUMO: -0.88981 factor:1 | 1 (-1.85546) | -1 | -1 |
| G: -5311.25950 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.65290 HOMO: -6.85999 LUMO: 0.07891 factor:1 | 1 (-2.02771) | -1 | -1 |
| G: -5311.25950 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.98152 HOMO: -7.08312 LUMO: -0.60137 factor:1 | 1 (-1.35632) | 1 | 1 |
| G: -5311.25950 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.05708 HOMO: -6.57699 LUMO: -0.68028 factor:1 | 1 (-1.43189) | -1 | -1 |
| G: -5311.25950 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.11439 HOMO: -6.09807 LUMO: -0.31837 factor:1 | 1 (-1.48920) | -1 | -1 |
| G: -5311.25950 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.17559 HOMO: -6.10624 LUMO: 0.14966 factor:1 | 1 (-1.55040) | -1 | -1 |
| G: -5311.25950 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.18280 HOMO: -6.77019 LUMO: -0.95784 factor:1 | 1 (-1.55761) | -1 | -1 |
| G: -5311.25950 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.11270 HOMO: -5.93208 LUMO: -0.44627 factor:1 | 1 (-1.48751) | -1 | -1 |
| G: -5311.25950 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.90410 HOMO: -6.12256 LUMO: -0.27756 factor:1 | 1 (-1.27891) | -1 | -1 |
| G: -5311.25950 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.87038 HOMO: -5.98106 LUMO: -0.37824 factor:1 | 1 (-1.24519) | -1 | -1 |
| G: -5311.25950 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.75283 HOMO: -7.06408 LUMO: -1.12927 factor:1 | 1 (-1.12764) | 1 | 1 |
| G: -5311.25950 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.90707 HOMO: -6.70761 LUMO: -0.98505 factor:1 | 1 (-1.28187) | -1 | -1 |
| G: -5311.25950 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.67103 HOMO: -7.00965 LUMO: -0.42722 factor:1 | 1 (-1.04584) | -1 | -1 |
| G: -5311.25950 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.89659 HOMO: -5.96201 LUMO: -0.59049 factor:1 | 1 (-1.27140) | -1 | -1 |
| G: -5311.25950 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.69893 HOMO: -6.34570 LUMO: -1.68438 factor:1 | 1 (-1.07373) | -1 | -1 |
| G: -5311.25950 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.93077 HOMO: -6.97156 LUMO: -1.85854 factor:1 | 1 (-1.30558) | -1 | -1 |
| G: -5311.25950 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.89904 HOMO: -5.91848 LUMO: -2.51433 factor:1 | 1 (-1.27385) | -1 | -1 |
| G: -5311.25950 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.77642 HOMO: -6.39195 LUMO: -1.66262 factor:1 | 1 (-1.15123) | -1 | -1 |
| G: -5311.25950 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.86100 HOMO: -6.50352 LUMO: 0.19592 factor:1 | 1 (-1.23581) | -1 | -1 |
| G: -5311.25950 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.59930 HOMO: -6.45998 LUMO: 0.34831 factor:1 | 1 (-0.97411) | -1 | -1 |
| G: -5311.25950 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.92663 HOMO: -7.05319 LUMO: 0.23402 factor:1 | 1 (-1.30144) | -1 | -1 |
| G: -5311.25950 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.68611 HOMO: -6.61237 LUMO: 0.18232 factor:1 | 1 (-1.06092) | -1 | -1 |
| G: -5311.25950 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.55683 HOMO: -6.57427 LUMO: 0.40545 factor:1 | 1 (-0.93164) | -1 | -1 |
| G: -5311.25950 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.51397 HOMO: -7.26544 LUMO: 0.41089 factor:1 | 1 (-0.88878) | 1 | 1 |
| G: -5311.25950 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.76355 HOMO: -6.26406 LUMO: -0.85444 factor:1 | 1 (-1.13836) | -1 | -1 |
| G: -5311.25950 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.57638 HOMO: -6.25318 LUMO: -0.79457 factor:1 | 1 (-1.95119) | -1 | -1 |
| G: -5311.25950 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.40958 HOMO: -6.68040 LUMO: 0.41089 factor:1 | 1 (-1.78439) | -1 | -1 |
| G: -5311.25950 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.54188 HOMO: -6.37835 LUMO: 0.37280 factor:1 | 1 (-1.91669) | -1 | -1 |
| G: -5311.25950 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.58384 HOMO: -6.56067 LUMO: 0.62858 factor:1 | 1 (-1.95865) | -1 | -1 |
| G: -5311.25950 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.70945 HOMO: -6.74026 LUMO: -0.04082 factor:1 | 1 (-2.08426) | -1 | -1 |
| G: -5311.25950 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.77786 HOMO: -6.53617 LUMO: 0.35103 factor:1 | 1 (-2.15267) | -1 | -1 |
| G: -5311.25950 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.55861 HOMO: -6.51985 LUMO: 0.25851 factor:1 | 1 (-1.93342) | -1 | -1 |
| G: -5311.25950 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.61418 HOMO: -6.58788 LUMO: -1.98371 factor:1 | 1 (-1.98899) | -1 | -1 |
| G: -5311.25950 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.50438 HOMO: -6.51441 LUMO: 0.29116 factor:1 | 1 (-1.87919) | -1 | -1 |
| G: -5311.25950 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.91176 HOMO: -6.81101 LUMO: 0.35647 factor:1 | 1 (-2.28657) | -1 | -1 |
| G: -5311.25950 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.48765 HOMO: -6.42733 LUMO: 0.10340 factor:1 | 1 (-1.86246) | -1 | -1 |
| G: -5311.25950 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.36862 HOMO: -6.70761 LUMO: 0.28028 factor:1 | 1 (-1.74343) | -1 | -1 |
| G: -5311.25950 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.25153 HOMO: -6.67495 LUMO: 0.01633 factor:1 | 1 (-1.62634) | -1 | -1 |
| G: -5311.25950 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.34509 HOMO: -6.75387 LUMO: 0.15510 factor:1 | 1 (-1.71990) | -1 | -1 |
| G: -5311.25950 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.64632 HOMO: -6.56067 LUMO: 0.35919 factor:1 | 1 (-2.02113) | -1 | -1 |
| G: -5311.25950 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.79182 HOMO: -7.16748 LUMO: 0.21497 factor:1 | 1 (-2.16662) | 1 | 1 |
| G: -5311.25950 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.57162 HOMO: -6.71849 LUMO: 0.26667 factor:1 | 1 (-1.94643) | -1 | -1 |
| G: -5311.25950 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.62871 HOMO: -6.69128 LUMO: 0.55783 factor:1 | 1 (-2.00352) | -1 | -1 |
| G: -5311.25950 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.87715 HOMO: -6.71305 LUMO: 0.45987 factor:1 | 1 (-2.25196) | -1 | -1 |
| G: -5311.25950 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.87813 HOMO: -5.90487 LUMO: -0.70750 factor:1 | 1 (-2.25294) | -1 | -1 |
| G: -5311.25950 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.57652 HOMO: -6.84638 LUMO: -0.72110 factor:1 | 1 (-1.95133) | -1 | -1 |
| G: -5311.25950 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.59940 HOMO: -6.66135 LUMO: -1.13471 factor:1 | 1 (-1.97421) | -1 | -1 |
| G: -5311.25950 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.48025 HOMO: -6.74026 LUMO: -0.64763 factor:1 | 1 (-1.85505) | -1 | -1 |
| G: -5311.25950 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.39891 HOMO: -6.69672 LUMO: -1.05036 factor:1 | 1 (-1.77372) | -1 | -1 |
| G: -5311.25950 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.41015 HOMO: -6.78924 LUMO: -1.03675 factor:1 | 1 (-1.78496) | -1 | -1 |
| G: -5311.25950 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.72392 HOMO: -6.81373 LUMO: -0.85988 factor:1 | 1 (-2.09873) | -1 | -1 |
| G: -5311.25950 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.55203 HOMO: -7.26544 LUMO: 0.91158 factor:1 | 1 (-1.92684) | 1 | 1 |
| G: -5311.25950 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.55497 HOMO: -6.64230 LUMO: -1.92929 factor:1 | 1 (-1.92978) | -1 | -1 |
| G: -5311.25950 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11578.15727 HOMO: -7.20830 LUMO: 0.11429 factor:1 | 1 (-2.53207) | 1 | 1 |
| G: -5311.25950 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11578.38769 HOMO: -7.17020 LUMO: 0.04898 factor:1 | 1 (-2.76250) | 1 | 1 |
| G: -5311.25950 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11578.98297 HOMO: -7.16476 LUMO: 0.04898 factor:1 | 1 (-3.35778) | 1 | 1 |
| G: -5311.25950 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.97255 HOMO: -6.59332 LUMO: -0.49253 factor:1 | 1 (-2.34736) | -1 | -1 |
| G: -5311.25950 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.96265 HOMO: -7.46953 LUMO: 0.84083 factor:1 | 1 (-2.33746) | 1 | 1 |
| G: -5311.25950 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11578.18861 HOMO: -7.39878 LUMO: 0.88709 factor:1 | 1 (-2.56342) | 1 | 1 |
| G: -5311.25950 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.99873 HOMO: -6.84094 LUMO: -0.61498 factor:1 | 1 (-2.37354) | -1 | -1 |
| G: -5311.25950 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.96820 HOMO: -6.03549 LUMO: -0.27211 factor:1 | 1 (-2.34301) | -1 | -1 |
| G: -5311.25950 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11578.19425 HOMO: -7.31170 LUMO: -0.64763 factor:1 | 1 (-2.56905) | 1 | 1 |
| G: -5311.25950 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.83141 HOMO: -6.88992 LUMO: -0.84627 factor:1 | 1 (-2.20622) | -1 | -1 |
| G: -5311.25950 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11578.98033 HOMO: -7.12666 LUMO: -0.09252 factor:1 | 1 (-3.35514) | 1 | 1 |
| G: -5311.25950 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11578.98218 HOMO: -6.70489 LUMO: -0.63675 factor:1 | 1 (-3.35699) | -1 | -1 |
| G: -5311.25950 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.79497 HOMO: -6.98788 LUMO: 0.86804 factor:1 | 1 (-2.16978) | -1 | -1 |
| G: -5311.25950 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11578.00496 HOMO: -6.80285 LUMO: -0.60954 factor:1 | 1 (-2.37977) | -1 | -1 |
| G: -5311.25950 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.93108 HOMO: -7.02054 LUMO: -0.74287 factor:1 | 1 (-2.30589) | -1 | -1 |
| G: -5311.25950 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.82882 HOMO: -7.03686 LUMO: -0.81090 factor:1 | 1 (-2.20363) | -1 | -1 |
| G: -5311.25950 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.58974 HOMO: -6.70489 LUMO: -1.00954 factor:1 | 1 (-1.96455) | -1 | -1 |
| G: -5311.25950 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11578.11101 HOMO: -7.69810 LUMO: 0.00544 factor:1 | 1 (-2.48581) | 1 | 1 |
| G: -5311.25950 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11578.38206 HOMO: -6.83550 LUMO: -0.11157 factor:1 | 1 (-2.75687) | -1 | -1 |
| G: -5311.25950 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11578.12611 HOMO: -6.76203 LUMO: -2.13609 factor:1 | 1 (-2.50092) | -1 | -1 |
| G: -5311.25950 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11578.10246 HOMO: -6.72121 LUMO: -2.62862 factor:1 | 1 (-2.47727) | -1 | -1 |
| G: -5311.25950 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.89930 HOMO: -6.48719 LUMO: -2.73474 factor:1 | 1 (-2.27411) | -1 | -1 |
| G: -5311.25950 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.80412 HOMO: -6.83006 LUMO: -0.00544 factor:1 | 1 (-1.17893) | -1 | -1 |
| G: -5311.25950 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.83515 HOMO: -6.84094 LUMO: -1.11022 factor:1 | 1 (-1.20995) | -1 | -1 |
| G: -5311.25950 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.02075 HOMO: -6.66951 LUMO: -1.23812 factor:1 | 1 (-1.39556) | -1 | -1 |
| G: -5311.25950 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.78886 HOMO: -6.78380 LUMO: -1.27894 factor:1 | 1 (-1.16367) | -1 | -1 |
| G: -5311.25950 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.73950 HOMO: -6.50352 LUMO: -0.56055 factor:1 | 1 (-1.11431) | -1 | -1 |
| G: -5311.25950 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.80244 HOMO: -7.77974 LUMO: -0.26395 factor:1 | 1 (-1.17725) | 1 | 1 |
| G: -5311.25950 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.59253 HOMO: -7.01510 LUMO: -1.64085 factor:1 | 1 (-0.96734) | -1 | -1 |
| G: -5311.25950 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.69710 HOMO: -6.59876 LUMO: -0.91158 factor:1 | 1 (-1.07191) | -1 | -1 |
| G: -5311.25950 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.88628 HOMO: -4.67219 LUMO: -0.67756 factor:1 | 1 (-1.26108) | -1 | -1 |
| G: -5311.25950 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.77851 HOMO: -6.70489 LUMO: -0.65579 factor:1 | 1 (-2.15332) | -1 | -1 |
| G: -5311.25950 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11578.60606 HOMO: -6.62325 LUMO: -0.60409 factor:1 | 1 (-2.98087) | -1 | -1 |
| G: -5311.25950 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.94219 HOMO: -6.20147 LUMO: 0.15238 factor:1 | 1 (-2.31700) | -1 | -1 |
| G: -5311.25950 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.83549 HOMO: -6.43549 LUMO: -0.07075 factor:1 | 1 (-2.21030) | -1 | -1 |
| G: -5311.25950 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.77712 HOMO: -7.02054 LUMO: 0.13061 factor:1 | 1 (-2.15193) | -1 | -1 |
| G: -5311.25950 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.57110 HOMO: -7.04503 LUMO: 0.30749 factor:1 | 1 (-1.94591) | -1 | -1 |
| G: -5311.25950 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.80442 HOMO: -6.74842 LUMO: -0.99594 factor:1 | 1 (-2.17922) | -1 | -1 |
| G: -5311.25950 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.61530 HOMO: -6.35658 LUMO: 0.41633 factor:1 | 1 (-1.99010) | -1 | -1 |
| G: -5311.25950 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.80771 HOMO: -6.79740 LUMO: 0.56872 factor:1 | 1 (-2.18252) | -1 | -1 |
| G: -5311.25950 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.65108 HOMO: -6.51713 LUMO: -0.05987 factor:1 | 1 (-2.02589) | -1 | -1 |
| G: -5311.25950 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.80096 HOMO: -6.68040 LUMO: 0.34558 factor:1 | 1 (-2.17577) | -1 | -1 |
| G: -5311.25950 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.76194 HOMO: -6.39740 LUMO: 0.50069 factor:1 | 1 (-2.13675) | -1 | -1 |
| G: -5311.25950 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.88070 HOMO: -6.91713 LUMO: -0.97145 factor:1 | 1 (-1.25551) | -1 | -1 |
| G: -5311.25950 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.90424 HOMO: -7.10761 LUMO: -0.27483 factor:1 | 1 (-1.27904) | 1 | -1 |
| G: -5311.25950 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.00598 HOMO: -6.98788 LUMO: 0.40273 factor:1 | 1 (-1.38079) | -1 | -1 |
| G: -5311.25950 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.12816 HOMO: -6.87087 LUMO: 0.28572 factor:1 | 1 (-1.50297) | -1 | -1 |
| G: -5311.25950 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.02026 HOMO: -7.36612 LUMO: -0.12245 factor:1 | 1 (-1.39507) | 1 | 1 |
| G: -5311.25950 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.92772 HOMO: -6.72938 LUMO: 0.33742 factor:1 | 1 (-1.30253) | -1 | -1 |
| G: -5311.25950 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.90870 HOMO: -7.32531 LUMO: 0.07619 factor:1 | 1 (-1.28351) | 1 | 1 |
| G: -5311.25950 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.04040 HOMO: -6.87087 LUMO: -0.08436 factor:1 | 1 (-1.41521) | -1 | -1 |
| G: -5311.25950 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.96747 HOMO: -6.67495 LUMO: 0.85988 factor:1 | 1 (-1.34228) | -1 | -1 |
| G: -5311.25950 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.68956 HOMO: -6.96339 LUMO: 0.65307 factor:1 | 1 (-1.06437) | -1 | -1 |
| G: -5311.25950 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.93128 HOMO: -6.58516 LUMO: -0.78641 factor:1 | 1 (-1.30609) | -1 | -1 |
| G: -5311.25950 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.76001 HOMO: -6.56883 LUMO: 0.44355 factor:1 | 1 (-1.13482) | -1 | -1 |
| G: -5311.25950 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.96421 HOMO: -6.68312 LUMO: 0.43538 factor:1 | 1 (-1.33902) | -1 | -1 |
| G: -5311.25950 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.01020 HOMO: -6.81917 LUMO: 0.20681 factor:1 | 1 (-1.38501) | -1 | -1 |
| G: -5311.25950 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.77836 HOMO: -6.91169 LUMO: 0.08163 factor:1 | 1 (-1.15316) | -1 | -1 |
| G: -5311.25950 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.00339 HOMO: -4.88444 LUMO: -0.49253 factor:1 | 1 (-1.37820) | -1 | -1 |
| G: -5311.25950 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.81721 HOMO: -6.42189 LUMO: 0.64763 factor:1 | 1 (-1.19202) | -1 | -1 |
| G: -5311.25950 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.98712 HOMO: -6.24501 LUMO: 0.55783 factor:1 | 1 (-1.36193) | -1 | -1 |
| G: -5311.25950 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.77871 HOMO: -6.41372 LUMO: 0.29388 factor:1 | 1 (-1.15352) | -1 | -1 |
| G: -5311.25950 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.09684 HOMO: -5.67902 LUMO: 1.77690 factor:1 | 1 (-1.47165) | -1 | -1 |
| G: -5311.25950 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.80837 HOMO: -6.55794 LUMO: 0.05170 factor:1 | 1 (-1.18318) | -1 | -1 |
| G: -5311.25950 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.56178 HOMO: -6.52801 LUMO: 0.25851 factor:1 | 1 (-0.93659) | -1 | -1 |
| G: -5311.25950 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.81928 HOMO: -7.08857 LUMO: 0.11157 factor:1 | 1 (-1.19409) | 1 | 1 |
| G: -5311.25950 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.04212 HOMO: -6.58243 LUMO: 0.75648 factor:1 | 1 (-1.41692) | -1 | -1 |
| G: -5311.25950 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.84208 HOMO: -7.22190 LUMO: 0.45171 factor:1 | 1 (-1.21689) | 1 | 1 |
| G: -5311.25950 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.93322 HOMO: -6.47087 LUMO: 0.00000 factor:1 | 1 (-1.30802) | -1 | -1 |
| G: -5311.25950 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.72227 HOMO: -6.78652 LUMO: 1.32247 factor:1 | 1 (-1.09708) | -1 | -1 |
| G: -5311.25950 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.04337 HOMO: -6.74026 LUMO: 1.45309 factor:1 | 1 (-1.41818) | -1 | -1 |
| G: -5311.25950 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.83278 HOMO: -6.69944 LUMO: 0.76464 factor:1 | 1 (-1.20759) | -1 | -1 |
| G: -5311.25950 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.79207 HOMO: -6.62325 LUMO: 0.64763 factor:1 | 1 (-1.16688) | -1 | -1 |
| G: -5311.25950 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.51941 HOMO: -6.45182 LUMO: 0.49253 factor:1 | 1 (-0.89422) | -1 | -1 |
| G: -5311.25950 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.88617 HOMO: -7.14843 LUMO: 0.62586 factor:1 | 1 (-1.26098) | 1 | 1 |
| G: -5311.25950 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.62926 HOMO: -6.87087 LUMO: 1.53200 factor:1 | 1 (-1.00407) | -1 | -1 |
| G: -5311.25950 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.44537 HOMO: -6.54978 LUMO: 0.45171 factor:1 | 1 (-0.82018) | -1 | -1 |
| G: -5311.25950 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.64423 HOMO: -6.63686 LUMO: 0.80001 factor:1 | 1 (-1.01904) | -1 | -1 |
| G: -5311.25950 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.80597 HOMO: -7.00693 LUMO: 1.56193 factor:1 | 1 (-1.18078) | -1 | -1 |
| G: -5311.25950 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.78347 HOMO: -6.02460 LUMO: 1.72792 factor:1 | 1 (-1.15828) | -1 | -1 |
| G: -5311.25950 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.83830 HOMO: -6.36746 LUMO: -1.20002 factor:1 | 1 (-1.21311) | -1 | -1 |
| G: -5311.25950 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.88540 HOMO: -7.26816 LUMO: -1.06397 factor:1 | 1 (-1.26021) | 1 | 1 |
| G: -5311.25950 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.79493 HOMO: -7.34707 LUMO: -1.09662 factor:1 | 1 (-1.16974) | 1 | 1 |
| G: -5311.25950 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.75939 HOMO: -7.93212 LUMO: -0.13606 factor:1 | 1 (-1.13420) | 1 | 1 |
| G: -5311.25950 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.79498 HOMO: -6.80285 LUMO: 0.58504 factor:1 | 1 (-1.16979) | -1 | -1 |
| G: -5311.25950 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.94500 HOMO: -7.12938 LUMO: 0.32926 factor:1 | 1 (-1.31981) | 1 | -1 |
| G: -5311.25950 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.10780 HOMO: -6.86815 LUMO: -1.30070 factor:1 | 1 (-1.48261) | -1 | -1 |
| G: -5311.25950 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.96911 HOMO: -6.99333 LUMO: -1.03947 factor:1 | 1 (-1.34392) | -1 | -1 |
| G: -5311.25950 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.01485 HOMO: -7.56749 LUMO: -0.11157 factor:1 | 1 (-1.38966) | 1 | 1 |
| G: -5311.25950 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.94728 HOMO: -7.57293 LUMO: -0.07891 factor:1 | 1 (-1.32209) | 1 | 1 |
| G: -5311.25950 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.91156 HOMO: -7.30626 LUMO: 0.27211 factor:1 | 1 (-1.28636) | 1 | 1 |
| G: -5311.25950 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.79046 HOMO: -7.77974 LUMO: 0.27211 factor:1 | 1 (-1.16527) | 1 | 1 |
| G: -5311.25950 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.98707 HOMO: -7.11578 LUMO: 0.19864 factor:1 | 1 (-1.36188) | 1 | 1 |
| G: -5311.25950 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.87191 HOMO: -7.71171 LUMO: 0.57688 factor:1 | 1 (-1.24672) | 1 | 1 |
| G: -5311.25950 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.15814 HOMO: -7.83688 LUMO: 0.37824 factor:1 | 1 (-1.53295) | 1 | 1 |
| G: -5311.25950 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.97226 HOMO: -6.94979 LUMO: -1.66534 factor:1 | 1 (-1.34707) | -1 | -1 |
| G: -5311.25950 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.93123 HOMO: -6.97156 LUMO: -1.13199 factor:1 | 1 (-1.30604) | -1 | -1 |
| G: -5311.25950 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.89789 HOMO: -6.91441 LUMO: -1.08301 factor:1 | 1 (-1.27270) | -1 | -1 |
| G: -5311.25950 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.04990 HOMO: -6.71849 LUMO: -0.74831 factor:1 | 1 (-1.42471) | -1 | -1 |
| G: -5311.25950 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.78608 HOMO: -7.09401 LUMO: -1.77690 factor:1 | 1 (-1.16089) | -1 | -1 |
| G: -5311.25950 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.96845 HOMO: -6.97156 LUMO: -1.45037 factor:1 | 1 (-1.34326) | -1 | -1 |
| G: -5311.25950 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.77359 HOMO: -7.22462 LUMO: -1.11295 factor:1 | 1 (-1.14840) | 1 | 1 |
| G: -5311.25950 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.96737 HOMO: -7.85321 LUMO: 0.16599 factor:1 | 1 (-1.34217) | 1 | 1 |
| G: -5311.25950 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.77528 HOMO: -7.71987 LUMO: 0.55511 factor:1 | 1 (-1.15009) | 1 | 1 |
| G: -5311.25950 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.98138 HOMO: -7.63551 LUMO: 0.14422 factor:1 | 1 (-1.35619) | 1 | 1 |
| G: -5311.25950 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.81403 HOMO: -6.98788 LUMO: -0.80546 factor:1 | 1 (-1.18884) | -1 | -1 |
| G: -5311.25950 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.43704 HOMO: -6.98788 LUMO: -1.16737 factor:1 | 1 (-0.81185) | -1 | -1 |
| G: -5311.25950 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.65620 HOMO: -6.56611 LUMO: -1.60819 factor:1 | 1 (-1.03101) | -1 | -1 |
| G: -5311.25950 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.51533 HOMO: -6.95251 LUMO: 0.66396 factor:1 | 1 (-0.89014) | -1 | -1 |
| G: -5311.25950 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.85691 HOMO: -7.35252 LUMO: 0.49797 factor:1 | 1 (-1.23172) | 1 | 1 |
| G: -5311.25950 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.58203 HOMO: -6.90897 LUMO: -0.81090 factor:1 | 1 (-0.95683) | -1 | -1 |
| G: -5311.25950 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.54646 HOMO: -7.04503 LUMO: -1.08301 factor:1 | 1 (-0.92127) | -1 | -1 |
| G: -5311.25950 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.38580 HOMO: -6.92530 LUMO: -1.29526 factor:1 | 1 (-0.76061) | -1 | -1 |
| G: -5311.25950 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.73158 HOMO: -6.93074 LUMO: -1.25444 factor:1 | 1 (-1.10639) | -1 | -1 |
| G: -5311.25950 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.91675 HOMO: -6.73482 LUMO: -0.62042 factor:1 | 1 (-1.29156) | -1 | -1 |
| G: -5311.25950 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.91068 HOMO: -7.67633 LUMO: 0.59593 factor:1 | 1 (-1.28549) | 1 | 1 |
| G: -5311.25950 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.89278 HOMO: -7.39061 LUMO: -0.19320 factor:1 | 1 (-1.26759) | 1 | 1 |
| G: -5311.25950 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.01104 HOMO: -7.55388 LUMO: -0.20136 factor:1 | 1 (-1.38585) | 1 | 1 |
| G: -5311.25950 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.03980 HOMO: -7.14027 LUMO: -0.99866 factor:1 | 1 (-1.41461) | 1 | 1 |
| G: -5311.25950 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.92524 HOMO: -6.75931 LUMO: -0.73199 factor:1 | 1 (-1.30005) | -1 | -1 |
| G: -5311.25950 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.88745 HOMO: -5.45044 LUMO: -0.18776 factor:1 | 1 (-1.26225) | -1 | -1 |
| G: -5311.25950 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.84663 HOMO: -6.70761 LUMO: -0.84083 factor:1 | 1 (-1.22144) | -1 | -1 |
| G: -5311.25950 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.82842 HOMO: -6.05453 LUMO: -1.06669 factor:1 | 1 (-1.20323) | -1 | -1 |
| G: -5311.25950 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.72116 HOMO: -6.86815 LUMO: -0.98233 factor:1 | 1 (-1.09597) | -1 | -1 |
| G: -5311.25950 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.69435 HOMO: -6.73210 LUMO: -0.95240 factor:1 | 1 (-1.06916) | -1 | -1 |
| G: -5311.25950 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.71814 HOMO: -5.89671 LUMO: -1.05036 factor:1 | 1 (-1.09295) | -1 | -1 |
| G: -5311.25950 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.92380 HOMO: -7.61102 LUMO: 0.33470 factor:1 | 1 (-1.29861) | 1 | 1 |
| G: -5311.25950 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.67005 HOMO: -7.51034 LUMO: 0.23674 factor:1 | 1 (-2.04485) | 1 | 1 |
| G: -5311.25950 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.79258 HOMO: -7.41510 LUMO: 0.62858 factor:1 | 1 (-2.16739) | 1 | 1 |
| G: -5311.25950 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.86420 HOMO: -6.76203 LUMO: -1.72792 factor:1 | 1 (-2.23901) | -1 | -1 |
| G: -5311.25950 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.47829 HOMO: -6.60420 LUMO: -0.45715 factor:1 | 1 (-1.85310) | -1 | -1 |
| G: -5311.25950 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.43505 HOMO: -6.59060 LUMO: -0.58232 factor:1 | 1 (-1.80986) | -1 | -1 |
| G: -5311.25950 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.44961 HOMO: -7.43687 LUMO: -0.76736 factor:1 | 1 (-1.82441) | 1 | 1 |
| G: -5311.25950 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.43265 HOMO: -6.08719 LUMO: -0.48708 factor:1 | 1 (-1.80746) | -1 | -1 |
| G: -5311.25950 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.28158 HOMO: -5.88854 LUMO: -0.05714 factor:1 | 1 (-1.65638) | -1 | -1 |
| G: -5311.25950 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.62134 HOMO: -7.34435 LUMO: -0.71838 factor:1 | 1 (-1.99615) | 1 | 1 |
| G: -5311.25950 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.47763 HOMO: -7.46408 LUMO: -0.63130 factor:1 | 1 (-1.85244) | 1 | 1 |
| G: -5311.25950 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.59516 HOMO: -7.00965 LUMO: -1.24900 factor:1 | 1 (-1.96997) | -1 | -1 |
| G: -5311.25950 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11578.21272 HOMO: -6.91169 LUMO: -0.88981 factor:1 | 1 (-2.58753) | -1 | -1 |
| G: -5311.25950 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11578.00401 HOMO: -6.78652 LUMO: -0.82178 factor:1 | 1 (-2.37882) | -1 | -1 |
| G: -5311.25950 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11578.02303 HOMO: -7.80423 LUMO: 0.87076 factor:1 | 1 (-2.39784) | 1 | 1 |
| G: -5311.25950 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11578.83529 HOMO: -6.97700 LUMO: -1.00954 factor:1 | 1 (-3.21010) | -1 | -1 |
| G: -5311.25950 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11578.98079 HOMO: -6.92530 LUMO: -0.88165 factor:1 | 1 (-3.35560) | -1 | -1 |
| G: -5311.25950 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.97506 HOMO: -7.14571 LUMO: -1.04492 factor:1 | 1 (-2.34987) | 1 | 1 |
| G: -5311.25950 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11578.15620 HOMO: -7.49674 LUMO: 0.34558 factor:1 | 1 (-2.53101) | 1 | 1 |
| G: -5311.25950 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.79141 HOMO: -6.44094 LUMO: -1.20819 factor:1 | 1 (-2.16622) | -1 | -1 |
| G: -5311.25950 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11578.04156 HOMO: -6.47359 LUMO: -1.14016 factor:1 | 1 (-2.41637) | -1 | -1 |
| G: -5311.25950 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.78665 HOMO: -6.61237 LUMO: -0.87076 factor:1 | 1 (-2.16145) | -1 | -1 |
| G: -5311.25950 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.80286 HOMO: -6.73754 LUMO: -1.09662 factor:1 | 1 (-2.17767) | -1 | -1 |
| G: -5311.25950 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.73818 HOMO: -6.97700 LUMO: 0.13061 factor:1 | 1 (-2.11299) | -1 | -1 |
| G: -5311.25950 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.59813 HOMO: -6.82734 LUMO: 0.59865 factor:1 | 1 (-1.97293) | -1 | -1 |
| G: -5311.25950 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.75245 HOMO: -6.86543 LUMO: -0.91430 factor:1 | 1 (-1.12726) | -1 | -1 |
| G: -5311.25950 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.96494 HOMO: -6.74298 LUMO: 0.28028 factor:1 | 1 (-1.33975) | -1 | -1 |
| G: -5311.25950 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.84187 HOMO: -6.75387 LUMO: 0.19592 factor:1 | 1 (-1.21668) | -1 | -1 |
| G: -5311.25950 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.90619 HOMO: -7.05591 LUMO: 0.10612 factor:1 | 1 (-1.28100) | -1 | -1 |
| G: -5311.25950 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.92399 HOMO: -6.86543 LUMO: 0.49253 factor:1 | 1 (-1.29880) | -1 | -1 |
| G: -5311.25950 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.91158 HOMO: -6.11440 LUMO: -1.12655 factor:1 | 1 (-1.28639) | -1 | -1 |
| G: -5311.25950 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.82829 HOMO: -6.77291 LUMO: -1.02859 factor:1 | 1 (-1.20310) | -1 | -1 |
| G: -5311.25950 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.77049 HOMO: -6.54978 LUMO: 0.29116 factor:1 | 1 (-1.14530) | -1 | -1 |
| G: -5311.25950 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.73539 HOMO: -7.18108 LUMO: 0.00000 factor:1 | 1 (-1.11020) | 1 | 1 |
| G: -5311.25950 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.56192 HOMO: -6.86271 LUMO: -1.15376 factor:1 | 1 (-0.93672) | -1 | -1 |
| G: -5311.25950 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.92170 HOMO: -6.78108 LUMO: -1.22723 factor:1 | 1 (-1.29651) | -1 | -1 |
| G: -5311.25950 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.75297 HOMO: -6.40828 LUMO: 0.02449 factor:1 | 1 (-1.12778) | -1 | -1 |
| G: -5311.25950 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.69699 HOMO: -6.43821 LUMO: 0.09796 factor:1 | 1 (-1.07180) | -1 | -1 |
| G: -5311.25950 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.98160 HOMO: -6.99877 LUMO: 0.40545 factor:1 | 1 (-1.35641) | -1 | -1 |
| G: -5311.25950 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.72401 HOMO: -6.68856 LUMO: 0.19320 factor:1 | 1 (-1.09882) | -1 | -1 |
| G: -5311.25950 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.75727 HOMO: -7.11034 LUMO: 0.31293 factor:1 | 1 (-1.13208) | 1 | 1 |
| G: -5311.25950 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.85528 HOMO: -6.92530 LUMO: -0.85444 factor:1 | 1 (-1.23009) | -1 | -1 |
| G: -5311.25950 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.76763 HOMO: -6.60148 LUMO: -0.59865 factor:1 | 1 (-1.14244) | -1 | -1 |
| G: -5311.25950 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.92845 HOMO: -6.72938 LUMO: 0.30749 factor:1 | 1 (-1.30326) | -1 | -1 |
| G: -5311.25950 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.62467 HOMO: -7.31170 LUMO: 0.06803 factor:1 | 1 (-0.99947) | 1 | 1 |
| G: -5311.25950 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.77778 HOMO: -7.09129 LUMO: -0.04626 factor:1 | 1 (-1.15259) | 1 | 1 |
| G: -5311.25950 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.50012 HOMO: -6.38379 LUMO: -0.76736 factor:1 | 1 (-0.87493) | -1 | -1 |
| G: -5311.25950 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.82051 HOMO: -6.13617 LUMO: -0.63947 factor:1 | 1 (-1.19531) | -1 | -1 |
| G: -5311.25950 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.71103 HOMO: -6.92258 LUMO: 0.37007 factor:1 | 1 (-1.08584) | -1 | -1 |
| G: -5311.25950 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.78891 HOMO: -6.35930 LUMO: 0.41361 factor:1 | 1 (-1.16372) | -1 | -1 |
| G: -5311.25950 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.69014 HOMO: -6.60420 LUMO: 0.26667 factor:1 | 1 (-1.06494) | -1 | -1 |
| G: -5311.25950 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.82894 HOMO: -6.04909 LUMO: 1.82588 factor:1 | 1 (-1.20375) | -1 | -1 |
| G: -5311.25950 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.67944 HOMO: -6.69672 LUMO: 1.72520 factor:1 | 1 (-1.05425) | -1 | -1 |
| G: -5311.25950 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.68910 HOMO: -6.50080 LUMO: 0.29116 factor:1 | 1 (-1.06391) | -1 | -1 |
| G: -5311.25950 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.54450 HOMO: -6.60692 LUMO: -0.43266 factor:1 | 1 (-0.91931) | -1 | -1 |
| G: -5311.25950 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.59109 HOMO: -6.93890 LUMO: 0.39729 factor:1 | 1 (-0.96590) | -1 | -1 |
| G: -5311.25950 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.88883 HOMO: -6.52801 LUMO: -0.47076 factor:1 | 1 (-1.26364) | -1 | -1 |
| G: -5311.25950 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.73686 HOMO: -6.41100 LUMO: 0.30477 factor:1 | 1 (-1.11167) | -1 | -1 |
| G: -5311.25950 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.79438 HOMO: -6.37291 LUMO: -0.80001 factor:1 | 1 (-1.16919) | -1 | -1 |
| G: -5311.25950 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.79302 HOMO: -6.51985 LUMO: 1.44765 factor:1 | 1 (-1.16783) | -1 | -1 |
| G: -5311.25950 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11578.18801 HOMO: -6.64774 LUMO: 0.04626 factor:1 | 1 (-2.56282) | -1 | -1 |
| G: -5311.25950 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11578.97167 HOMO: -6.65863 LUMO: 0.29933 factor:1 | 1 (-3.34648) | -1 | -1 |
| G: -5311.25950 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.98662 HOMO: -7.09673 LUMO: 0.28300 factor:1 | 1 (-2.36143) | 1 | 1 |
| G: -5311.25950 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11578.13373 HOMO: -6.57155 LUMO: -1.11567 factor:1 | 1 (-2.50854) | -1 | -1 |
| G: -5311.25950 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11578.14733 HOMO: -6.38379 LUMO: -0.60681 factor:1 | 1 (-2.52214) | -1 | -1 |
| G: -5311.25950 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11578.00404 HOMO: -6.60148 LUMO: 0.18232 factor:1 | 1 (-2.37885) | -1 | -1 |
| G: -5311.25950 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.68978 HOMO: -6.96067 LUMO: -0.52246 factor:1 | 1 (-1.06459) | -1 | -1 |
| G: -5311.25950 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.74864 HOMO: -6.57427 LUMO: -0.84627 factor:1 | 1 (-1.12345) | -1 | -1 |
| G: -5311.25950 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.75269 HOMO: -6.59332 LUMO: -0.98233 factor:1 | 1 (-1.12750) | -1 | -1 |
| G: -5311.25950 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.55775 HOMO: -6.20692 LUMO: -0.27483 factor:1 | 1 (-0.93256) | -1 | -1 |
| G: -5311.25950 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.61917 HOMO: -6.81373 LUMO: 0.74559 factor:1 | 1 (-0.99398) | -1 | -1 |
| G: -5311.25950 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.43552 HOMO: -6.60420 LUMO: 0.54695 factor:1 | 1 (-0.81033) | -1 | -1 |
| G: -5311.25950 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.42877 HOMO: -6.58788 LUMO: -0.31021 factor:1 | 1 (-0.80358) | -1 | -1 |
| G: -5311.25950 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.81506 HOMO: -6.72938 LUMO: 0.64763 factor:1 | 1 (-1.18987) | -1 | -1 |
| G: -5311.25950 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.65373 HOMO: -6.86815 LUMO: 0.32109 factor:1 | 1 (-1.02854) | -1 | -1 |
| G: -5311.25950 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.64442 HOMO: -6.63141 LUMO: 0.18776 factor:1 | 1 (-1.01923) | -1 | -1 |
| G: -5311.25950 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.74826 HOMO: -7.18653 LUMO: 0.09524 factor:1 | 1 (-1.12307) | 1 | 1 |
| G: -5311.25950 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11578.46035 HOMO: -6.83550 LUMO: 0.03537 factor:1 | 1 (-2.83515) | -1 | -1 |
| G: -5311.25950 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.67075 HOMO: -7.47769 LUMO: 0.40817 factor:1 | 1 (-2.04556) | 1 | 1 |
| G: -5311.25950 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.71456 HOMO: -6.57971 LUMO: -0.63675 factor:1 | 1 (-2.08937) | -1 | -1 |
| G: -5311.25950 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.74607 HOMO: -6.74842 LUMO: -0.16327 factor:1 | 1 (-2.12088) | -1 | -1 |
| G: -5311.25950 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.74722 HOMO: -7.07224 LUMO: 0.61770 factor:1 | 1 (-2.12203) | 1 | 1 |
| G: -5311.25950 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.60368 HOMO: -6.83006 LUMO: 0.54695 factor:1 | 1 (-1.97849) | -1 | -1 |
| G: -5311.25950 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.80047 HOMO: -6.60148 LUMO: 1.23540 factor:1 | 1 (-2.17528) | -1 | -1 |
| G: -5312.42844 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.03352 HOMO: -6.99061 LUMO: 0.41089 factor:1 | 1 (-0.23938) | -1 | -1 |
| G: -5312.42844 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.84902 HOMO: -6.63686 LUMO: 0.85172 factor:1 | 1 (-0.05489) | -1 | -1 |
| G: -5312.42844 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.57944 HOMO: -6.50624 LUMO: 0.12517 factor:1 | -1 (0.21470) | -1 | -1 |
| G: -5312.42844 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11578.44220 HOMO: -6.35658 LUMO: 0.36463 factor:1 | 1 (-1.64806) | -1 | -1 |
| G: -5312.42844 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11578.06807 HOMO: -6.34570 LUMO: 0.65035 factor:1 | 1 (-1.27393) | -1 | -1 |
| G: -5312.42844 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11579.01581 HOMO: -6.63141 LUMO: 1.25717 factor:1 | 1 (-2.22167) | -1 | -1 |
| G: -5312.42844 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11578.14426 HOMO: -6.91441 LUMO: 1.32792 factor:1 | 1 (-1.35012) | -1 | -1 |
| G: -5312.42844 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11578.29803 HOMO: -7.15387 LUMO: 0.64219 factor:1 | 1 (-1.50389) | 1 | 1 |
| G: -5312.42844 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.87095 HOMO: -7.17836 LUMO: 0.60409 factor:1 | 1 (-1.07681) | 1 | 1 |
| G: -5312.42844 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.91870 HOMO: -6.92258 LUMO: 0.49525 factor:1 | 1 (-1.12456) | -1 | -1 |
| G: -5312.42844 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.90734 HOMO: -6.31032 LUMO: 0.48708 factor:1 | 1 (-0.11320) | -1 | -1 |
| G: -5312.42844 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.31279 HOMO: -6.49808 LUMO: 0.31021 factor:1 | 1 (-0.51865) | -1 | -1 |
| G: -5312.42844 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.94470 HOMO: -6.48447 LUMO: 0.37552 factor:1 | 1 (-0.15056) | -1 | -1 |
| G: -5312.42844 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.26729 HOMO: -6.66135 LUMO: -1.08301 factor:1 | 1 (-0.47315) | -1 | -1 |
| G: -5312.42844 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.20982 HOMO: -6.33481 LUMO: -0.51974 factor:1 | 1 (-0.41568) | -1 | -1 |
| G: -5312.42844 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.44933 HOMO: -6.76475 LUMO: -0.15238 factor:1 | 1 (-0.65520) | -1 | -1 |
| G: -5312.42844 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.61638 HOMO: -6.93346 LUMO: -0.10885 factor:1 | 1 (-0.82225) | -1 | -1 |
| G: -5312.42844 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.80545 HOMO: -7.19741 LUMO: 0.73199 factor:1 | 1 (-1.01131) | 1 | 1 |
| G: -5312.42844 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.94529 HOMO: -6.82734 LUMO: 0.88437 factor:1 | 1 (-1.15115) | -1 | -1 |
| G: -5312.42844 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.65973 HOMO: -7.01237 LUMO: 0.02721 factor:1 | 1 (-0.86559) | -1 | -1 |
| G: -5312.42844 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.23591 HOMO: -6.39195 LUMO: 1.46941 factor:1 | 1 (-0.44178) | -1 | -1 |
| G: -5312.42844 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.16650 HOMO: -6.53890 LUMO: 1.32792 factor:1 | 1 (-0.37236) | -1 | -1 |
| G: -5312.42844 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.81999 HOMO: -6.82734 LUMO: 1.98099 factor:1 | 1 (-0.02585) | -1 | -1 |
| G: -5312.42844 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.19684 HOMO: -6.74570 LUMO: 1.68983 factor:1 | 1 (-0.40270) | -1 | -1 |
| G: -5312.42844 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.95011 HOMO: -6.41100 LUMO: 1.39050 factor:1 | 1 (-0.15598) | -1 | -1 |
| G: -5312.42844 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.75980 HOMO: -5.92664 LUMO: 1.65989 factor:1 | -1 (0.03434) | -1 | -1 |
| G: -5312.42844 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.04078 HOMO: -6.07630 LUMO: 1.54833 factor:1 | 1 (-0.24664) | -1 | -1 |
| G: -5312.42844 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.98805 HOMO: -6.45998 LUMO: 0.68573 factor:1 | 1 (-0.19391) | -1 | -1 |
| G: -5312.42844 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11578.40693 HOMO: -6.52801 LUMO: 0.41361 factor:1 | 1 (-1.61279) | -1 | -1 |
| G: -5312.42844 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.71807 HOMO: -6.77564 LUMO: 0.42178 factor:1 | 1 (-0.92394) | -1 | -1 |
| G: -5312.42844 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.81658 HOMO: -6.56339 LUMO: 1.65717 factor:1 | 1 (-1.02244) | -1 | -1 |
| G: -5312.42844 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11578.02926 HOMO: -5.85861 LUMO: 1.90752 factor:1 | 1 (-1.23512) | -1 | -1 |
| G: -5312.42844 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11578.34372 HOMO: -6.77019 LUMO: -2.48440 factor:1 | 1 (-1.54958) | -1 | -1 |
| G: -5312.42844 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11578.21977 HOMO: -6.53890 LUMO: -1.82588 factor:1 | 1 (-1.42563) | -1 | -1 |
| G: -5312.42844 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11578.26497 HOMO: -6.50352 LUMO: -1.66806 factor:1 | 1 (-1.47083) | -1 | -1 |
| G: -5312.42844 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11578.14668 HOMO: -6.90625 LUMO: 0.43538 factor:1 | 1 (-1.35254) | -1 | -1 |
| G: -5312.42844 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.03763 HOMO: -6.85455 LUMO: 0.53062 factor:1 | 1 (-0.24349) | -1 | -1 |
| G: -5312.42844 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.87120 HOMO: -6.49536 LUMO: 0.31021 factor:1 | 1 (-0.07706) | -1 | -1 |
| G: -5312.42844 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.07972 HOMO: -4.97696 LUMO: -0.09252 factor:1 | 1 (-0.28558) | -1 | -1 |
| G: -5312.42844 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11578.43659 HOMO: -5.31166 LUMO: 0.34286 factor:1 | 1 (-1.64245) | -1 | -1 |
| G: -5312.42844 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.90921 HOMO: -6.42461 LUMO: 0.74287 factor:1 | 1 (-1.11507) | -1 | -1 |
| G: -5312.42844 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.80221 HOMO: -6.59604 LUMO: 0.62858 factor:1 | 1 (-1.00807) | -1 | -1 |
| G: -5312.42844 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.90619 HOMO: -6.45998 LUMO: -0.61770 factor:1 | 1 (-1.11205) | -1 | -1 |
| G: -5312.42844 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11578.00703 HOMO: -6.75659 LUMO: -0.34014 factor:1 | 1 (-1.21289) | -1 | -1 |
| G: -5312.42844 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.87946 HOMO: -6.63958 LUMO: 0.36191 factor:1 | 1 (-1.08533) | -1 | -1 |
| G: -5312.42844 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.13657 HOMO: -5.92936 LUMO: -0.67484 factor:1 | 1 (-0.34243) | -1 | -1 |
| G: -5312.42844 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.05120 HOMO: -5.67630 LUMO: 1.80956 factor:1 | 1 (-0.25707) | -1 | -1 |
| G: -5312.42844 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.94410 HOMO: -6.50352 LUMO: -0.78369 factor:1 | 1 (-0.14996) | -1 | -1 |
| G: -5312.42844 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.12138 HOMO: -6.35930 LUMO: -0.75648 factor:1 | 1 (-0.32724) | -1 | -1 |
| G: -5312.42844 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.04282 HOMO: -6.74298 LUMO: 0.48980 factor:1 | 1 (-0.24868) | -1 | -1 |
| G: -5312.42844 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.03874 HOMO: -6.85183 LUMO: 0.15510 factor:1 | 1 (-0.24460) | -1 | -1 |
| G: -5312.42844 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.05523 HOMO: -6.90897 LUMO: 0.26123 factor:1 | 1 (-0.26109) | -1 | -1 |
| G: -5312.42844 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.92949 HOMO: -6.85999 LUMO: 0.47892 factor:1 | 1 (-0.13535) | -1 | -1 |
| G: -5312.42844 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.12590 HOMO: -6.69944 LUMO: 0.57416 factor:1 | 1 (-0.33176) | -1 | -1 |
| G: -5312.42844 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.08603 HOMO: -6.74026 LUMO: 0.69933 factor:1 | 1 (-0.29190) | -1 | -1 |
| G: -5312.42844 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.07700 HOMO: -6.52801 LUMO: 0.75376 factor:1 | 1 (-0.28286) | -1 | -1 |
| G: -5312.42844 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.84032 HOMO: -7.05863 LUMO: 0.44627 factor:1 | 1 (-0.04618) | -1 | -1 |
| G: -5312.42844 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.02666 HOMO: -6.96339 LUMO: 0.48164 factor:1 | 1 (-0.23252) | -1 | -1 |
| G: -5312.42844 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.85101 HOMO: -6.95795 LUMO: 0.44355 factor:1 | 1 (-0.05687) | -1 | -1 |
| G: -5312.42844 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.06329 HOMO: -6.36746 LUMO: 0.58777 factor:1 | 1 (-0.26915) | -1 | -1 |
| G: -5312.42844 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11579.05184 HOMO: -6.69400 LUMO: 0.40545 factor:1 | 1 (-2.25770) | -1 | -1 |
| G: -5312.42844 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11578.24889 HOMO: -6.30760 LUMO: -0.66668 factor:1 | 1 (-1.45475) | -1 | -1 |
| G: -5312.42844 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11578.30391 HOMO: -6.53617 LUMO: -0.64491 factor:1 | 1 (-1.50977) | -1 | -1 |
| G: -5312.42844 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.91966 HOMO: -6.80829 LUMO: 0.17415 factor:1 | 1 (-0.12553) | -1 | -1 |
| G: -5312.42844 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.90990 HOMO: -6.80285 LUMO: 0.73471 factor:1 | 1 (-0.11576) | -1 | -1 |
| G: -5312.42844 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.92821 HOMO: -6.43821 LUMO: 0.21769 factor:1 | 1 (-0.13407) | -1 | -1 |
| G: -5312.42844 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.01300 HOMO: -6.98788 LUMO: 0.10885 factor:1 | 1 (-0.21886) | -1 | -1 |
| G: -5312.42844 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11578.36530 HOMO: -7.15115 LUMO: 0.40817 factor:1 | 1 (-1.57116) | 1 | 1 |
| G: -5312.42844 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.72863 HOMO: -6.00011 LUMO: -0.98505 factor:1 | 1 (-0.93449) | -1 | -1 |
| G: -5312.42844 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.93634 HOMO: -6.16882 LUMO: -0.77825 factor:1 | 1 (-1.14220) | -1 | -1 |
| G: -5312.42844 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.90281 HOMO: -6.30760 LUMO: 0.34831 factor:1 | 1 (-1.10867) | -1 | -1 |
| G: -5312.42844 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.89751 HOMO: -6.64502 LUMO: 0.63403 factor:1 | 1 (-1.10337) | -1 | -1 |
| G: -5312.42844 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.93692 HOMO: -6.93618 LUMO: 0.96600 factor:1 | 1 (-0.14278) | -1 | -1 |
| G: -5312.42844 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.06900 HOMO: -6.45182 LUMO: 0.16327 factor:1 | 1 (-0.27486) | -1 | -1 |
| G: -5312.42844 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.92396 HOMO: -6.99605 LUMO: 0.20953 factor:1 | 1 (-0.12983) | -1 | -1 |
| G: -5312.42844 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.15140 HOMO: -6.72665 LUMO: 0.32654 factor:1 | 1 (-0.35726) | -1 | -1 |
| G: -5312.42844 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.18797 HOMO: -6.38379 LUMO: 0.45443 factor:1 | 1 (-0.39383) | -1 | -1 |
| G: -5312.42844 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.46615 HOMO: -6.65318 LUMO: 0.04354 factor:1 | 1 (-0.67201) | -1 | -1 |
| G: -5312.42844 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.13589 HOMO: -6.94707 LUMO: -1.68438 factor:1 | 1 (-0.34175) | -1 | -1 |
| G: -5312.42844 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.33159 HOMO: -6.71849 LUMO: 0.15783 factor:1 | 1 (-0.53745) | -1 | -1 |
| G: -5312.42844 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.22342 HOMO: -6.97156 LUMO: 0.43266 factor:1 | 1 (-0.42929) | -1 | -1 |
| G: -5312.42844 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.13433 HOMO: -6.91441 LUMO: -0.54695 factor:1 | 1 (-0.34020) | -1 | -1 |
| G: -5312.42844 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.29834 HOMO: -6.74842 LUMO: -0.76192 factor:1 | 1 (-0.50420) | -1 | -1 |
| G: -5312.42844 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.22571 HOMO: -6.70489 LUMO: 0.19048 factor:1 | 1 (-0.43157) | -1 | -1 |
| G: -5312.42844 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.12233 HOMO: -7.25728 LUMO: 0.33470 factor:1 | 1 (-0.32820) | 1 | -1 |
| G: -5312.42844 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.17338 HOMO: -6.96339 LUMO: 0.55511 factor:1 | 1 (-0.37925) | -1 | -1 |
| G: -5312.42844 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.99752 HOMO: -6.77564 LUMO: 0.72382 factor:1 | 1 (-0.20338) | -1 | -1 |
| G: -5312.42844 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.02682 HOMO: -6.75387 LUMO: 0.39729 factor:1 | 1 (-0.23268) | -1 | -1 |
| G: -5312.42844 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.08987 HOMO: -7.00149 LUMO: 0.06531 factor:1 | 1 (-0.29573) | -1 | -1 |
| G: -5312.42844 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.17028 HOMO: -7.09945 LUMO: 0.33470 factor:1 | 1 (-0.37614) | 1 | 1 |
| G: -5312.42844 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.28193 HOMO: -7.20830 LUMO: 0.59593 factor:1 | 1 (-0.48779) | 1 | 1 |
| G: -5312.42844 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.68126 HOMO: -6.40556 LUMO: 0.56600 factor:1 | 1 (-0.88712) | -1 | -1 |
| G: -5312.42844 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.87073 HOMO: -6.77291 LUMO: 0.73471 factor:1 | 1 (-1.07659) | -1 | -1 |
| G: -5312.42844 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.64139 HOMO: -6.65046 LUMO: 0.09796 factor:1 | 1 (-0.84725) | -1 | -1 |
| G: -5312.42844 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.89272 HOMO: -6.95795 LUMO: 0.22313 factor:1 | 1 (-1.09858) | -1 | -1 |
| G: -5312.42844 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.62999 HOMO: -6.85727 LUMO: 0.04626 factor:1 | 1 (-0.83585) | -1 | -1 |
| G: -5312.42844 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.95459 HOMO: -7.27360 LUMO: 0.42178 factor:1 | 1 (-1.16046) | 1 | 1 |
| G: -5312.42844 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.05490 HOMO: -6.78924 LUMO: -0.13334 factor:1 | 1 (-0.26077) | -1 | -1 |
| G: -5312.42844 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.99806 HOMO: -6.63141 LUMO: 0.38368 factor:1 | 1 (-0.20392) | -1 | -1 |
| G: -5312.42844 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.06497 HOMO: -6.92258 LUMO: 0.39184 factor:1 | 1 (-0.27083) | -1 | -1 |
| G: -5312.42844 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.12217 HOMO: -6.19331 LUMO: -0.46804 factor:1 | 1 (-0.32803) | -1 | -1 |
| G: -5312.42844 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.08105 HOMO: -7.26544 LUMO: -0.05442 factor:1 | 1 (-0.28692) | 1 | 1 |
| G: -5312.42844 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.15738 HOMO: -7.09401 LUMO: 0.30749 factor:1 | 1 (-0.36324) | 1 | 1 |
| G: -5312.42844 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.20478 HOMO: -6.14705 LUMO: -0.88709 factor:1 | 1 (-0.41065) | -1 | -1 |
| G: -5312.42844 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.15923 HOMO: -6.53617 LUMO: -0.28572 factor:1 | 1 (-0.36510) | -1 | -1 |
| G: -5312.42844 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.50906 HOMO: -6.37291 LUMO: -0.67212 factor:1 | 1 (-0.71492) | -1 | -1 |
| G: -5312.42844 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.31507 HOMO: -6.65591 LUMO: 0.03810 factor:1 | 1 (-0.52093) | -1 | -1 |
| G: -5312.42844 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.22440 HOMO: -7.11034 LUMO: 0.75103 factor:1 | 1 (-0.43027) | 1 | 1 |
| G: -5312.42844 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.26255 HOMO: -6.85183 LUMO: -0.05987 factor:1 | 1 (-0.46842) | -1 | -1 |
| G: -5312.42844 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.25654 HOMO: -6.70761 LUMO: -0.05442 factor:1 | 1 (-0.46240) | -1 | -1 |
| G: -5312.42844 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.12729 HOMO: -6.23413 LUMO: 0.06259 factor:1 | 1 (-0.33315) | -1 | -1 |
| G: -5312.42844 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.22789 HOMO: -6.55794 LUMO: 0.74015 factor:1 | 1 (-0.43375) | -1 | -1 |
| G: -5312.42844 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.18367 HOMO: -7.27905 LUMO: 0.26939 factor:1 | 1 (-0.38953) | 1 | 1 |
| G: -5312.42844 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.06089 HOMO: -6.34842 LUMO: -0.86804 factor:1 | 1 (-0.26675) | -1 | -1 |
| G: -5312.42844 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.70915 HOMO: -6.27222 LUMO: 1.46125 factor:1 | 1 (-0.91501) | -1 | -1 |
| G: -5312.42844 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.97250 HOMO: -6.65046 LUMO: 2.04902 factor:1 | 1 (-1.17836) | -1 | -1 |
| G: -5312.42844 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.98733 HOMO: -7.11850 LUMO: -1.14016 factor:1 | 1 (-1.19319) | 1 | -1 |
| G: -5312.42844 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.89506 HOMO: -6.88720 LUMO: -1.20274 factor:1 | 1 (-1.10092) | -1 | -1 |
| G: -5312.42844 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11578.00728 HOMO: -6.69400 LUMO: -0.31565 factor:1 | 1 (-1.21314) | -1 | -1 |
| G: -5312.42844 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.81571 HOMO: -6.95523 LUMO: -1.55377 factor:1 | 1 (-1.02157) | -1 | -1 |
| G: -5312.42844 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.80836 HOMO: -6.41372 LUMO: -0.83539 factor:1 | 1 (-1.01422) | -1 | -1 |
| G: -5312.42844 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.17161 HOMO: -6.13889 LUMO: -0.90070 factor:1 | 1 (-0.37748) | -1 | -1 |
| G: -5312.42844 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.31047 HOMO: -6.44366 LUMO: -0.55511 factor:1 | 1 (-0.51634) | -1 | -1 |
| G: -5312.42844 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.22168 HOMO: -6.10079 LUMO: -0.71022 factor:1 | 1 (-0.42755) | -1 | -1 |
| G: -5312.42844 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.13526 HOMO: -6.90353 LUMO: -0.64763 factor:1 | 1 (-0.34112) | -1 | -1 |
| G: -5312.42844 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.58749 HOMO: -6.65046 LUMO: -0.82450 factor:1 | 1 (-0.79335) | -1 | -1 |
| G: -5312.42844 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.71002 HOMO: -6.81645 LUMO: -0.85444 factor:1 | 1 (-0.91588) | -1 | -1 |
| G: -5312.42844 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.74716 HOMO: -6.20692 LUMO: 1.30887 factor:1 | 1 (-0.95302) | -1 | -1 |
| G: -5312.42844 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.88082 HOMO: -5.96201 LUMO: 1.33880 factor:1 | 1 (-1.08669) | -1 | -1 |
| G: -5312.42844 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.70433 HOMO: -6.52529 LUMO: 1.58914 factor:1 | 1 (-0.91019) | -1 | -1 |
| G: -5312.42844 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.57698 HOMO: -6.58516 LUMO: 1.97555 factor:1 | 1 (-0.78284) | -1 | -1 |
| G: -5312.42844 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.69598 HOMO: -6.84366 LUMO: 0.15783 factor:1 | 1 (-0.90184) | -1 | -1 |
| G: -5312.42844 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.75065 HOMO: -6.45726 LUMO: 0.42994 factor:1 | 1 (-0.95651) | -1 | -1 |
| G: -5312.42844 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.51976 HOMO: -6.75387 LUMO: 0.14422 factor:1 | 1 (-0.72562) | -1 | -1 |
| G: -5312.42844 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.58476 HOMO: -6.69944 LUMO: 1.79051 factor:1 | 1 (-0.79063) | -1 | -1 |
| G: -5312.42844 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.88763 HOMO: -6.59876 LUMO: 1.90208 factor:1 | 1 (-1.09349) | -1 | -1 |
| G: -5312.42844 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.91780 HOMO: -7.05863 LUMO: 1.20819 factor:1 | 1 (-1.12367) | -1 | -1 |
| G: -5312.42844 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.67233 HOMO: -6.54978 LUMO: 2.01636 factor:1 | 1 (-0.87819) | -1 | -1 |
| G: -5312.42844 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.71426 HOMO: -5.52119 LUMO: 1.95106 factor:1 | 1 (-0.92013) | -1 | -1 |
| G: -5312.42844 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11578.38712 HOMO: -6.53617 LUMO: 1.60275 factor:1 | 1 (-1.59298) | -1 | -1 |
| G: -5312.42844 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11579.11660 HOMO: -6.11440 LUMO: 1.89119 factor:1 | 1 (-2.32246) | -1 | -1 |
| G: -5312.42844 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11578.42862 HOMO: -7.31986 LUMO: 0.48708 factor:1 | 1 (-1.63448) | 1 | 1 |
| G: -5312.42844 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.91500 HOMO: -6.76475 LUMO: -0.75648 factor:1 | 1 (-1.12086) | -1 | -1 |
| G: -5312.42844 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.91029 HOMO: -6.76747 LUMO: -1.06941 factor:1 | 1 (-1.11616) | -1 | -1 |
| G: -5312.42844 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11578.02831 HOMO: -6.87087 LUMO: 0.72927 factor:1 | 1 (-1.23417) | -1 | -1 |
| G: -5312.42844 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11578.37950 HOMO: -7.00965 LUMO: 0.02177 factor:1 | 1 (-1.58536) | -1 | -1 |
| G: -5312.42844 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11578.22298 HOMO: -6.54706 LUMO: -0.03265 factor:1 | 1 (-1.42884) | -1 | -1 |
| G: -5312.42844 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11578.33262 HOMO: -6.62325 LUMO: -0.63675 factor:1 | 1 (-1.53848) | -1 | -1 |
| G: -5312.42844 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.01199 HOMO: -7.03414 LUMO: -1.24084 factor:1 | 1 (-0.21785) | -1 | -1 |
| G: -5312.42844 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.90432 HOMO: -7.04503 LUMO: -0.10068 factor:1 | 1 (-0.11018) | -1 | -1 |
| G: -5312.42844 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.92502 HOMO: -6.67223 LUMO: 0.03537 factor:1 | 1 (-0.13089) | -1 | -1 |
| G: -5312.42844 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.15861 HOMO: -6.82734 LUMO: 0.58777 factor:1 | 1 (-0.36447) | -1 | -1 |
| G: -5312.42844 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11578.59148 HOMO: -6.84366 LUMO: 0.46531 factor:1 | 1 (-1.79734) | -1 | -1 |
| G: -5312.42844 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.94219 HOMO: -7.03959 LUMO: -1.15104 factor:1 | 1 (-1.14805) | -1 | -1 |
| G: -5312.42844 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.91201 HOMO: -6.91169 LUMO: -0.41361 factor:1 | 1 (-1.11787) | -1 | -1 |
| G: -5312.42844 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.96205 HOMO: -7.10217 LUMO: -0.44627 factor:1 | 1 (-1.16791) | 1 | 1 |
| G: -5312.42844 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.99577 HOMO: -6.88176 LUMO: -0.19592 factor:1 | 1 (-0.20164) | -1 | -1 |
| G: -5312.42844 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.90045 HOMO: -7.21374 LUMO: -0.46531 factor:1 | 1 (-0.10631) | 1 | 1 |
| G: -5312.42844 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.05071 HOMO: -6.54978 LUMO: 0.16871 factor:1 | 1 (-0.25658) | -1 | -1 |
| G: -5312.42844 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.38057 HOMO: -6.71305 LUMO: -0.13061 factor:1 | 1 (-0.58643) | -1 | -1 |
| G: -5312.42844 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.16176 HOMO: -6.74842 LUMO: -0.36191 factor:1 | 1 (-0.36763) | -1 | -1 |
| G: -5312.42844 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.94481 HOMO: -6.74570 LUMO: -0.09796 factor:1 | 1 (-0.15067) | -1 | -1 |
| G: -5312.42844 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.86679 HOMO: -6.93890 LUMO: -0.27211 factor:1 | 1 (-0.07265) | -1 | -1 |
| G: -5312.42844 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.16906 HOMO: -6.88720 LUMO: -0.18776 factor:1 | 1 (-0.37492) | -1 | -1 |
| G: -5312.42844 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.93460 HOMO: -6.74842 LUMO: 0.02993 factor:1 | 1 (-0.14047) | -1 | -1 |
| G: -5312.42844 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.21706 HOMO: -6.70216 LUMO: 0.01361 factor:1 | 1 (-0.42292) | -1 | -1 |
| G: -5312.42844 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.88181 HOMO: -6.90625 LUMO: 0.00544 factor:1 | 1 (-0.08768) | -1 | -1 |
| G: -5312.42844 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.90274 HOMO: -6.18243 LUMO: 0.25851 factor:1 | 1 (-0.10860) | -1 | -1 |
| G: -5312.42844 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.03129 HOMO: -6.32937 LUMO: -0.20953 factor:1 | 1 (-0.23715) | -1 | -1 |
| G: -5312.42844 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.05471 HOMO: -6.78108 LUMO: 0.00544 factor:1 | 1 (-0.26058) | -1 | -1 |
| G: -5312.42844 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.27061 HOMO: -5.97562 LUMO: 0.28572 factor:1 | 1 (-0.47647) | -1 | -1 |
| G: -5312.42844 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.14631 HOMO: -5.97290 LUMO: -0.18504 factor:1 | 1 (-0.35217) | -1 | -1 |
| G: -5312.42844 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.00557 HOMO: -6.12800 LUMO: 0.42178 factor:1 | 1 (-0.21143) | -1 | -1 |
| G: -5312.42844 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.11578 HOMO: -6.24229 LUMO: -0.00816 factor:1 | 1 (-0.32164) | -1 | -1 |
| G: -5312.42844 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.31690 HOMO: -6.61781 LUMO: 0.12789 factor:1 | 1 (-0.52276) | -1 | -1 |
| G: -5312.42844 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.00252 HOMO: -6.70489 LUMO: 0.14694 factor:1 | 1 (-0.20838) | -1 | -1 |
| G: -5312.42844 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.12522 HOMO: -6.86543 LUMO: -0.21225 factor:1 | 1 (-0.33108) | -1 | -1 |
| G: -5312.42844 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.01020 HOMO: -6.90081 LUMO: -0.20136 factor:1 | 1 (-0.21606) | -1 | -1 |
| G: -5312.42844 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.08067 HOMO: -7.12938 LUMO: -0.25851 factor:1 | 1 (-0.28654) | 1 | 1 |
| G: -5312.42844 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.06127 HOMO: -6.93074 LUMO: -0.26667 factor:1 | 1 (-0.26713) | -1 | -1 |
| G: -5312.42844 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.15706 HOMO: -7.00421 LUMO: -0.31021 factor:1 | 1 (-0.36292) | -1 | -1 |
| G: -5312.42844 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.65244 HOMO: -7.10761 LUMO: -0.17415 factor:1 | 1 (-0.85830) | 1 | 1 |
| G: -5312.42844 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.76240 HOMO: -8.21240 LUMO: 0.05987 factor:1 | 1 (-0.96826) | 1 | 1 |
| G: -5312.42844 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.95296 HOMO: -7.14843 LUMO: -0.46531 factor:1 | 1 (-1.15882) | 1 | -1 |
| G: -5312.42844 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.53309 HOMO: -6.80829 LUMO: -0.29933 factor:1 | 1 (-0.73895) | -1 | -1 |
| G: -5312.42844 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.78809 HOMO: -6.84094 LUMO: -0.53606 factor:1 | 1 (-0.99395) | -1 | -1 |
| G: -5312.42844 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.64134 HOMO: -6.81917 LUMO: -0.26667 factor:1 | 1 (-0.84720) | -1 | -1 |
| G: -5312.42844 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11578.02616 HOMO: -6.85727 LUMO: -1.20002 factor:1 | 1 (-1.23202) | -1 | -1 |
| G: -5312.42844 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.81554 HOMO: -6.39468 LUMO: -1.06941 factor:1 | 1 (-1.02141) | -1 | -1 |
| G: -5312.42844 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.89647 HOMO: -6.00827 LUMO: -1.94017 factor:1 | 1 (-1.10233) | -1 | -1 |
| G: -5312.42844 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.96118 HOMO: -6.80829 LUMO: 0.18504 factor:1 | 1 (-1.16704) | -1 | -1 |
| G: -5312.42844 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.97621 HOMO: -6.54434 LUMO: -0.95784 factor:1 | 1 (-0.18207) | -1 | -1 |
| G: -5312.42844 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.02353 HOMO: -6.45454 LUMO: -0.07347 factor:1 | 1 (-0.22939) | -1 | -1 |
| G: -5312.42844 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.14419 HOMO: -5.33887 LUMO: 1.11839 factor:1 | 1 (-0.35005) | -1 | -1 |
| G: -5312.42844 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.08429 HOMO: -5.75249 LUMO: 0.70477 factor:1 | 1 (-0.29016) | -1 | -1 |
| G: -5312.42844 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.99433 HOMO: -5.64092 LUMO: 0.87076 factor:1 | 1 (-0.20019) | -1 | -1 |
| G: -5312.42844 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.78886 HOMO: -5.14295 LUMO: 1.06124 factor:1 | -1 (0.00528) | -1 | -1 |
| G: -5312.42844 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.83689 HOMO: -5.05043 LUMO: 1.21091 factor:1 | 1 (-0.04275) | -1 | -1 |
| G: -5312.42844 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.91945 HOMO: -5.05588 LUMO: 1.02859 factor:1 | 1 (-0.12531) | -1 | -1 |
| G: -5312.42844 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.97485 HOMO: -5.76337 LUMO: 0.79457 factor:1 | 1 (-0.18071) | -1 | -1 |
| G: -5312.42844 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.14516 HOMO: -5.01506 LUMO: 1.00138 factor:1 | 1 (-0.35103) | -1 | -1 |
| G: -5312.42844 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.85101 HOMO: -4.84363 LUMO: 1.53744 factor:1 | 1 (-0.05687) | -1 | -1 |
| G: -5312.42844 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.75041 HOMO: -5.17833 LUMO: 1.45309 factor:1 | -1 (0.04373) | -1 | -1 |
| G: -5312.42844 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.88045 HOMO: -5.13751 LUMO: 0.51157 factor:1 | 1 (-0.08631) | -1 | -1 |
| G: -5312.42844 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.78189 HOMO: -5.56473 LUMO: 0.32109 factor:1 | -1 (0.01225) | -1 | -1 |
| G: -5312.42844 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.06329 HOMO: -4.69941 LUMO: 1.14016 factor:1 | 1 (-0.26915) | -1 | -1 |
| G: -5312.42844 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.90037 HOMO: -4.49260 LUMO: 1.86398 factor:1 | 1 (-0.10623) | -1 | -1 |
| G: -5312.42844 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.05787 HOMO: -4.32117 LUMO: 1.68438 factor:1 | 1 (-0.26373) | -1 | -1 |
| G: -5312.42844 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11578.95440 HOMO: -4.44906 LUMO: 1.37690 factor:1 | 1 (-2.16026) | -1 | -1 |
| G: -5312.42844 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11578.00401 HOMO: -4.62049 LUMO: 1.34968 factor:1 | 1 (-1.20987) | -1 | -1 |
| G: -5312.42844 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11578.22633 HOMO: -4.59600 LUMO: 1.58370 factor:1 | 1 (-1.43219) | -1 | -1 |
| G: -5312.42844 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11578.35074 HOMO: -4.98785 LUMO: 1.46669 factor:1 | 1 (-1.55660) | -1 | -1 |
| G: -5312.42844 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.72037 HOMO: -5.06676 LUMO: 1.27349 factor:1 | -1 (0.07377) | -1 | -1 |
| G: -5312.42844 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.85237 HOMO: -5.09125 LUMO: 1.13471 factor:1 | 1 (-0.05823) | -1 | -1 |
| G: -5312.42844 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.97158 HOMO: -4.84635 LUMO: 1.33608 factor:1 | 1 (-0.17745) | -1 | -1 |
| G: -5312.42844 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.81248 HOMO: -4.94431 LUMO: 1.18370 factor:1 | 1 (-0.01834) | -1 | -1 |
| G: -5312.42844 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.69759 HOMO: -4.92526 LUMO: 1.39867 factor:1 | -1 (0.09655) | -1 | -1 |
| G: -5312.42844 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11578.44543 HOMO: -5.71983 LUMO: 0.60137 factor:1 | 1 (-1.65130) | -1 | -1 |
| G: -5312.42844 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.65519 HOMO: -5.10486 LUMO: 1.05580 factor:1 | 1 (-0.86105) | -1 | -1 |
| G: -5312.42844 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.75337 HOMO: -5.20282 LUMO: 1.01226 factor:1 | 1 (-0.95923) | -1 | -1 |
| G: -5312.42844 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.83933 HOMO: -4.98513 LUMO: 1.53744 factor:1 | 1 (-1.04519) | -1 | -1 |
| G: -5312.42844 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.96779 HOMO: -5.67085 LUMO: 0.17687 factor:1 | 1 (-1.17365) | -1 | -1 |
| G: -5312.42844 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.95855 HOMO: -5.87222 LUMO: 0.12517 factor:1 | 1 (-0.16441) | -1 | -1 |
| G: -5312.42844 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.21649 HOMO: -5.20826 LUMO: 0.91702 factor:1 | 1 (-0.42235) | -1 | -1 |
| G: -5312.42844 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.91822 HOMO: -5.94569 LUMO: 0.63130 factor:1 | 1 (-0.12408) | -1 | -1 |
| G: -5312.42844 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.98994 HOMO: -5.35792 LUMO: 0.91430 factor:1 | 1 (-1.19580) | -1 | -1 |
| G: -5312.42844 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.99277 HOMO: -5.36336 LUMO: 1.44220 factor:1 | 1 (-1.19863) | -1 | -1 |
| G: -5312.42844 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.87527 HOMO: -5.83412 LUMO: 0.71294 factor:1 | 1 (-1.08114) | -1 | -1 |
| G: -5312.42844 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.86178 HOMO: -4.97696 LUMO: 1.72792 factor:1 | 1 (-1.06764) | -1 | -1 |
| G: -5312.42844 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.93106 HOMO: -5.55929 LUMO: 0.23130 factor:1 | 1 (-1.13692) | -1 | -1 |
| G: -5312.42844 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11578.52731 HOMO: -5.71167 LUMO: 0.47348 factor:1 | 1 (-1.73317) | -1 | -1 |
| G: -5312.42844 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.20008 HOMO: -7.31986 LUMO: -2.54699 factor:1 | 1 (-0.40594) | -1 | -1 |
| G: -5312.42844 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11578.21245 HOMO: -5.34704 LUMO: 1.19730 factor:1 | 1 (-1.41831) | -1 | -1 |
| G: -5312.42844 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11578.08701 HOMO: -5.45860 LUMO: 0.80818 factor:1 | 1 (-1.29287) | -1 | -1 |
| G: -5312.42844 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.99424 HOMO: -5.12663 LUMO: 1.20274 factor:1 | 1 (-1.20010) | -1 | -1 |
| G: -5312.42844 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.67342 HOMO: -5.37153 LUMO: 1.05580 factor:1 | 1 (-0.87928) | -1 | -1 |
| G: -5312.42844 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.91821 HOMO: -5.47221 LUMO: 0.97961 factor:1 | 1 (-1.12408) | -1 | -1 |
| G: -5312.42844 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11578.06709 HOMO: -5.06948 LUMO: 1.12111 factor:1 | 1 (-1.27295) | -1 | -1 |
| G: -5312.42844 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.82091 HOMO: -5.19737 LUMO: 1.25444 factor:1 | 1 (-1.02677) | -1 | -1 |
| G: -5312.42844 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.66515 HOMO: -5.27901 LUMO: 1.00682 factor:1 | 1 (-0.87101) | -1 | -1 |
| G: -5312.42844 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.37486 HOMO: -5.38513 LUMO: 0.49253 factor:1 | 1 (-0.58072) | -1 | -1 |
| G: -5312.42844 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.47339 HOMO: -5.12390 LUMO: 1.22995 factor:1 | 1 (-0.67925) | -1 | -1 |
| G: -5312.42844 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.45910 HOMO: -5.31438 LUMO: 0.70205 factor:1 | 1 (-0.66496) | -1 | -1 |
| G: -5312.42844 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.26756 HOMO: -5.17561 LUMO: 1.04492 factor:1 | 1 (-0.47342) | -1 | -1 |
| G: -5312.42844 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.88371 HOMO: -4.94431 LUMO: 1.52656 factor:1 | 1 (-1.08957) | -1 | -1 |
| G: -5312.42844 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.62332 HOMO: -5.13751 LUMO: 0.93879 factor:1 | 1 (-0.82919) | -1 | -1 |
| G: -5312.42844 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.62354 HOMO: -5.49942 LUMO: 0.97689 factor:1 | 1 (-0.82940) | -1 | -1 |
| G: -5312.42844 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.48607 HOMO: -5.79058 LUMO: 0.53879 factor:1 | 1 (-0.69193) | -1 | -1 |
| G: -5312.42844 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.54626 HOMO: -5.36881 LUMO: 1.56465 factor:1 | 1 (-0.75212) | -1 | -1 |
| G: -5312.42844 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.46640 HOMO: -4.67492 LUMO: 1.32792 factor:1 | 1 (-0.67226) | -1 | -1 |
| G: -5312.42844 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.40193 HOMO: -4.60145 LUMO: 1.19458 factor:1 | 1 (-0.60779) | -1 | -1 |
| G: -5312.42844 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.17673 HOMO: -4.49260 LUMO: 1.60547 factor:1 | 1 (-0.38259) | -1 | -1 |
| G: -5312.42844 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.32386 HOMO: -4.65043 LUMO: 1.34696 factor:1 | 1 (-0.52972) | -1 | -1 |
| G: -5312.42844 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.29080 HOMO: -4.77560 LUMO: 1.35241 factor:1 | 1 (-0.49666) | -1 | -1 |
| G: -5312.42844 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.73803 HOMO: -4.94431 LUMO: 1.17825 factor:1 | -1 (0.05611) | -1 | -1 |
| G: -5312.42844 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.10696 HOMO: -4.87084 LUMO: 1.41771 factor:1 | 1 (-0.31282) | -1 | -1 |
| G: -5312.42844 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.27080 HOMO: -5.34432 LUMO: 1.16737 factor:1 | 1 (-0.47666) | -1 | -1 |
| G: -5312.42844 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.31456 HOMO: -4.94975 LUMO: 1.67622 factor:1 | 1 (-0.52042) | -1 | -1 |
| G: -5312.42844 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.44906 HOMO: -4.81369 LUMO: 1.14288 factor:1 | 1 (-0.65492) | -1 | -1 |
| G: -5312.42844 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.46435 HOMO: -5.22459 LUMO: 0.29660 factor:1 | 1 (-0.67022) | -1 | -1 |
| G: -5312.42844 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.85116 HOMO: -5.21642 LUMO: 0.37824 factor:1 | 1 (-1.05703) | -1 | -1 |
| G: -5312.42844 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11578.06088 HOMO: -5.00417 LUMO: 1.01226 factor:1 | 1 (-1.26674) | -1 | -1 |
| G: -5312.42844 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11578.02202 HOMO: -5.46677 LUMO: 0.10612 factor:1 | 1 (-1.22789) | -1 | -1 |
| G: -5312.42844 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11578.21381 HOMO: -5.51303 LUMO: 0.54151 factor:1 | 1 (-1.41967) | -1 | -1 |
| G: -5312.42844 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.77380 HOMO: -5.63004 LUMO: 0.17960 factor:1 | 1 (-0.97966) | -1 | -1 |
| G: -5312.42844 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11578.00850 HOMO: -4.79193 LUMO: 1.12111 factor:1 | 1 (-1.21436) | -1 | -1 |
| G: -5312.42844 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.95089 HOMO: -5.43411 LUMO: 0.45987 factor:1 | 1 (-1.15676) | -1 | -1 |
| G: -5312.42844 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11578.06075 HOMO: -7.06135 LUMO: -2.13881 factor:1 | 1 (-1.26661) | 1 | 1 |
| G: -5312.42844 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.89399 HOMO: -5.33071 LUMO: 1.14016 factor:1 | 1 (-1.09986) | -1 | -1 |
| G: -5312.42844 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11578.14146 HOMO: -7.12394 LUMO: -0.03810 factor:1 | 1 (-1.34732) | 1 | 1 |
| G: -5312.42844 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.70452 HOMO: -7.20558 LUMO: -2.50889 factor:1 | 1 (-0.91038) | 1 | 1 |
| G: -5312.42844 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.86997 HOMO: -7.26816 LUMO: -2.11432 factor:1 | 1 (-1.07583) | 1 | 1 |
| G: -5312.42844 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.77571 HOMO: -7.89674 LUMO: 0.31021 factor:1 | 1 (-0.98157) | 1 | 1 |
| G: -5312.42844 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.81361 HOMO: -7.26544 LUMO: 0.22858 factor:1 | 1 (-1.01947) | 1 | 1 |
| G: -5312.42844 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.86338 HOMO: -7.12666 LUMO: -0.02449 factor:1 | 1 (-1.06924) | 1 | 1 |
| G: -5312.42844 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11578.22701 HOMO: -7.68722 LUMO: 0.71838 factor:1 | 1 (-1.43287) | 1 | 1 |
| G: -5312.42844 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11578.04143 HOMO: -6.86271 LUMO: -0.96056 factor:1 | 1 (-1.24729) | -1 | -1 |
| G: -5312.42844 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11578.00494 HOMO: -7.07496 LUMO: -1.11839 factor:1 | 1 (-1.21080) | 1 | 1 |
| G: -5312.42844 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.23273 HOMO: -7.06952 LUMO: -2.08439 factor:1 | 1 (-0.43859) | 1 | 1 |
| G: -5312.42844 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.31940 HOMO: -6.60965 LUMO: -2.11977 factor:1 | 1 (-0.52526) | -1 | -1 |
| G: -5312.42844 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.90151 HOMO: -6.87360 LUMO: -1.85854 factor:1 | 1 (-0.10738) | -1 | -1 |
| G: -5312.42844 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.00786 HOMO: -7.67089 LUMO: -0.24762 factor:1 | 1 (-0.21372) | 1 | 1 |
| G: -5312.42844 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.24511 HOMO: -6.45726 LUMO: -1.86398 factor:1 | 1 (-0.45097) | -1 | -1 |
| G: -5312.42844 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.43682 HOMO: -6.91713 LUMO: 0.33198 factor:1 | 1 (-0.64268) | -1 | -1 |
| G: -5312.42844 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.83966 HOMO: -6.83278 LUMO: 0.26667 factor:1 | 1 (-0.04552) | -1 | -1 |
| G: -5312.42844 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.07820 HOMO: -6.89264 LUMO: -1.00682 factor:1 | 1 (-0.28406) | -1 | -1 |
| G: -5312.42844 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.27589 HOMO: -6.57427 LUMO: 0.22041 factor:1 | 1 (-0.48175) | -1 | -1 |
| G: -5312.42844 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.84099 HOMO: -7.52123 LUMO: -0.01905 factor:1 | 1 (-1.04685) | 1 | 1 |
| G: -5312.42844 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.84602 HOMO: -7.37429 LUMO: -0.08980 factor:1 | 1 (-1.05188) | 1 | 1 |
| G: -5312.42844 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.77715 HOMO: -7.28449 LUMO: -0.26395 factor:1 | 1 (-0.98301) | 1 | 1 |
| G: -5312.42844 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.77601 HOMO: -6.79740 LUMO: -0.60954 factor:1 | 1 (-0.98187) | -1 | -1 |
| G: -5312.42844 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.84099 HOMO: -7.12666 LUMO: -0.60681 factor:1 | 1 (-1.04685) | 1 | 1 |
| G: -5312.42844 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.76071 HOMO: -6.96611 LUMO: -0.30477 factor:1 | 1 (-0.96658) | -1 | -1 |
| G: -5312.42844 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.82929 HOMO: -7.08040 LUMO: -0.31293 factor:1 | 1 (-1.03515) | 1 | 1 |
| G: -5312.42844 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.83998 HOMO: -6.78924 LUMO: -0.73743 factor:1 | 1 (-1.04584) | -1 | -1 |
| G: -5312.42844 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11578.06382 HOMO: -7.57293 LUMO: -1.11295 factor:1 | 1 (-1.26968) | 1 | 1 |
| G: -5312.42844 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11578.05656 HOMO: -7.15932 LUMO: -0.23130 factor:1 | 1 (-1.26242) | 1 | 1 |
| G: -5312.42844 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.78877 HOMO: -7.48585 LUMO: -0.10068 factor:1 | 1 (-0.99463) | 1 | 1 |
| G: -5312.42844 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.94172 HOMO: -7.17020 LUMO: -0.26123 factor:1 | 1 (-1.14759) | 1 | 1 |
| G: -5312.42844 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.96847 HOMO: -7.43143 LUMO: -0.16055 factor:1 | 1 (-1.17433) | 1 | 1 |
| G: -5312.42844 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.95070 HOMO: -7.14843 LUMO: -0.10612 factor:1 | 1 (-1.15657) | 1 | 1 |
| G: -5312.42844 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.86142 HOMO: -6.95523 LUMO: -0.22585 factor:1 | 1 (-1.06728) | -1 | -1 |
| G: -5312.42844 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.97636 HOMO: -7.06680 LUMO: -0.51974 factor:1 | 1 (-1.18223) | 1 | 1 |
| G: -5312.42844 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.71573 HOMO: -6.80829 LUMO: -0.64763 factor:1 | 1 (-0.92160) | -1 | -1 |
| G: -5312.42844 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11578.05544 HOMO: -7.13210 LUMO: -0.48164 factor:1 | 1 (-1.26130) | 1 | 1 |
| G: -5312.42844 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11578.06317 HOMO: -7.16204 LUMO: -0.45715 factor:1 | 1 (-1.26903) | 1 | 1 |
| G: -5312.42844 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11578.09218 HOMO: -7.15115 LUMO: -0.43266 factor:1 | 1 (-1.29804) | 1 | 1 |
| G: -5312.42844 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.77130 HOMO: -7.15932 LUMO: -2.52794 factor:1 | 1 (-0.97716) | -1 | -1 |
| G: -5312.42844 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.76115 HOMO: -7.21102 LUMO: -2.65311 factor:1 | 1 (-0.96701) | -1 | -1 |
| G: -5312.42844 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11578.03054 HOMO: -6.57427 LUMO: -2.78645 factor:1 | 1 (-1.23640) | -1 | -1 |
| G: -5312.42844 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.76855 HOMO: -6.40828 LUMO: -3.23815 factor:1 | 1 (-0.97441) | -1 | -1 |
| G: -5312.42844 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.89979 HOMO: -7.71987 LUMO: -0.20953 factor:1 | 1 (-1.10565) | 1 | 1 |
| G: -5312.42844 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.75244 HOMO: -7.47769 LUMO: -0.43810 factor:1 | 1 (-0.95830) | 1 | 1 |
| G: -5312.42844 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.68357 HOMO: -6.68040 LUMO: -2.22589 factor:1 | 1 (-0.88943) | -1 | -1 |
| G: -5312.42844 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.96059 HOMO: -6.92802 LUMO: -1.99187 factor:1 | 1 (-0.16645) | -1 | -1 |
| G: -5312.42844 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.28223 HOMO: -7.73620 LUMO: 0.01633 factor:1 | 1 (-0.48809) | 1 | 1 |
| G: -5312.42844 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.07545 HOMO: -7.28721 LUMO: -0.18504 factor:1 | 1 (-0.28131) | 1 | 1 |
| G: -5312.42844 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.03052 HOMO: -7.49674 LUMO: -0.19864 factor:1 | 1 (-0.23639) | 1 | 1 |
| G: -5312.42844 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.86180 HOMO: -7.10489 LUMO: -2.56331 factor:1 | 1 (-1.06767) | -1 | -1 |
| G: -5312.42844 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.72137 HOMO: -7.36612 LUMO: 0.16055 factor:1 | 1 (-0.92723) | 1 | 1 |
| G: -5312.42844 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11578.10442 HOMO: -7.67633 LUMO: 0.33198 factor:1 | 1 (-1.31028) | 1 | 1 |
| G: -5312.42844 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.94834 HOMO: -7.07768 LUMO: -0.27483 factor:1 | 1 (-1.15420) | 1 | 1 |
| G: -5312.42844 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.93908 HOMO: -7.32531 LUMO: 0.05442 factor:1 | 1 (-1.14495) | 1 | 1 |
| G: -5312.42844 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11578.05239 HOMO: -6.79740 LUMO: -1.21635 factor:1 | 1 (-1.25825) | -1 | -1 |
| G: -5312.42844 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.78537 HOMO: -7.14027 LUMO: 0.12517 factor:1 | 1 (-0.99123) | 1 | -1 |
| G: -5312.42844 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.85157 HOMO: -7.17292 LUMO: 0.16871 factor:1 | 1 (-1.05743) | 1 | -1 |
| G: -5312.42844 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11578.03854 HOMO: -7.08312 LUMO: -1.38778 factor:1 | 1 (-1.24440) | 1 | 1 |
| G: -5312.42844 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11578.06763 HOMO: -6.75387 LUMO: -1.88031 factor:1 | 1 (-1.27349) | -1 | -1 |
| G: -5312.42844 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11578.09294 HOMO: -7.07768 LUMO: -1.25717 factor:1 | 1 (-1.29880) | 1 | 1 |
| G: -5312.42844 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.93631 HOMO: -6.46543 LUMO: -1.14016 factor:1 | 1 (-1.14217) | -1 | -1 |
| G: -5312.42844 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.77212 HOMO: -7.37973 LUMO: -0.45987 factor:1 | 1 (-0.97798) | 1 | 1 |
| G: -5312.42844 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.61630 HOMO: -7.46408 LUMO: 0.03265 factor:1 | 1 (-0.82216) | 1 | 1 |
| G: -5312.42844 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.80455 HOMO: -7.96477 LUMO: -0.19864 factor:1 | 1 (-1.01041) | 1 | 1 |
| G: -5312.42844 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.87865 HOMO: -6.93890 LUMO: -1.11839 factor:1 | 1 (-1.08451) | -1 | -1 |
| G: -5312.42844 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.74014 HOMO: -7.06408 LUMO: -1.08846 factor:1 | 1 (-0.94600) | 1 | 1 |
| G: -5312.42844 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.56972 HOMO: -7.14027 LUMO: -0.33470 factor:1 | 1 (-0.77558) | 1 | 1 |
| G: -5312.42844 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.44552 HOMO: -7.38245 LUMO: 0.10885 factor:1 | 1 (-0.65139) | 1 | 1 |
| G: -5312.42844 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.59935 HOMO: -7.59470 LUMO: -1.21363 factor:1 | 1 (-0.80521) | 1 | 1 |
| G: -5312.42844 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.52329 HOMO: -7.23279 LUMO: -1.23812 factor:1 | 1 (-0.72916) | 1 | 1 |
| G: -5312.42844 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.71383 HOMO: -6.90897 LUMO: 0.23402 factor:1 | 1 (-0.91969) | -1 | -1 |
| G: -5312.42844 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.42596 HOMO: -7.36340 LUMO: -0.17143 factor:1 | 1 (-0.63182) | 1 | 1 |
| G: -5312.42844 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.65685 HOMO: -6.61781 LUMO: -0.01361 factor:1 | 1 (-0.86271) | -1 | -1 |
| G: -5312.42844 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.50610 HOMO: -6.80013 LUMO: 0.38368 factor:1 | 1 (-0.71196) | -1 | -1 |
| G: -5312.42844 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.60893 HOMO: -6.72121 LUMO: -0.95512 factor:1 | 1 (-0.81479) | -1 | -1 |
| G: -5312.42844 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.82452 HOMO: -6.24773 LUMO: -0.69933 factor:1 | 1 (-1.03039) | -1 | -1 |
| G: -5312.42844 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.53584 HOMO: -6.56883 LUMO: 0.14694 factor:1 | 1 (-0.74170) | -1 | -1 |
| G: -5312.42844 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.48803 HOMO: -6.51441 LUMO: -1.27621 factor:1 | 1 (-0.69389) | -1 | -1 |
| G: -5312.42844 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.43894 HOMO: -6.91986 LUMO: -1.16737 factor:1 | 1 (-0.64480) | -1 | -1 |
| G: -5312.42844 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.72343 HOMO: -6.17971 LUMO: -0.65307 factor:1 | 1 (-0.92930) | -1 | -1 |
| G: -5312.42844 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.63081 HOMO: -7.22462 LUMO: 0.04354 factor:1 | 1 (-0.83667) | 1 | 1 |
| G: -5312.42844 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.70928 HOMO: -7.16204 LUMO: -0.23674 factor:1 | 1 (-0.91515) | 1 | 1 |
| G: -5312.42844 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.74349 HOMO: -6.81645 LUMO: -0.19320 factor:1 | 1 (-0.94935) | -1 | -1 |
| G: -5312.42844 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.83481 HOMO: -6.69400 LUMO: 0.04082 factor:1 | 1 (-1.04067) | -1 | -1 |
| G: -5312.42844 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11578.05411 HOMO: -6.63141 LUMO: -0.22858 factor:1 | 1 (-1.25997) | -1 | -1 |
| G: -5312.42844 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.79761 HOMO: -6.92258 LUMO: -1.11295 factor:1 | 1 (-1.00347) | -1 | -1 |
| G: -5312.42844 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.76428 HOMO: -6.60148 LUMO: -1.13744 factor:1 | 1 (-0.97014) | -1 | -1 |
| G: -5312.42844 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.75108 HOMO: -6.78108 LUMO: -0.82450 factor:1 | 1 (-0.95694) | -1 | -1 |
| G: -5312.42844 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.91136 HOMO: -7.05591 LUMO: -0.97145 factor:1 | 1 (-1.11722) | -1 | -1 |
| G: -5312.42844 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.70488 HOMO: -6.65318 LUMO: -1.26261 factor:1 | 1 (-0.91074) | -1 | -1 |
| G: -5312.42844 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.78934 HOMO: -6.98244 LUMO: -0.98233 factor:1 | 1 (-0.99520) | -1 | -1 |
| G: -5312.42844 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.48343 HOMO: -7.11850 LUMO: -0.99594 factor:1 | 1 (-0.68929) | 1 | 1 |
| G: -5312.42844 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.43818 HOMO: -6.64230 LUMO: -0.93879 factor:1 | 1 (-0.64404) | -1 | -1 |
| G: -5312.42844 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.54229 HOMO: -6.62053 LUMO: -1.22451 factor:1 | 1 (-0.74815) | -1 | -1 |
| G: -5312.42844 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.43543 HOMO: -7.02598 LUMO: -0.85172 factor:1 | 1 (-0.64129) | -1 | -1 |
| G: -5312.42844 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.34990 HOMO: -7.06680 LUMO: -0.89253 factor:1 | 1 (-0.55577) | 1 | 1 |
| G: -5312.42844 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.39061 HOMO: -7.17292 LUMO: 0.00272 factor:1 | 1 (-0.59647) | 1 | 1 |
| G: -5312.42844 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.64136 HOMO: -7.03142 LUMO: -0.35103 factor:1 | 1 (-0.84723) | -1 | -1 |
| G: -5312.42844 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.42732 HOMO: -6.96884 LUMO: -0.09796 factor:1 | 1 (-0.63318) | -1 | -1 |
| G: -5312.42844 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.73405 HOMO: -6.56339 LUMO: -0.99322 factor:1 | 1 (-0.93991) | -1 | -1 |
| G: -5312.42844 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.48950 HOMO: -7.08857 LUMO: -0.17687 factor:1 | 1 (-0.69536) | 1 | 1 |
| G: -5312.42844 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.33015 HOMO: -7.05863 LUMO: -0.22041 factor:1 | 1 (-0.53601) | -1 | -1 |
| G: -5312.42844 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.27763 HOMO: -7.15115 LUMO: -0.17960 factor:1 | 1 (-0.48349) | 1 | 1 |
| G: -5312.42844 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.17774 HOMO: -6.67495 LUMO: -0.96600 factor:1 | 1 (-0.38360) | -1 | -1 |
| G: -5312.42844 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.93550 HOMO: -6.74026 LUMO: -1.79867 factor:1 | 1 (-0.14136) | -1 | -1 |
| G: -5312.42844 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.42231 HOMO: -6.73482 LUMO: -1.78235 factor:1 | 1 (-0.62817) | -1 | -1 |
| G: -5312.42844 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.22381 HOMO: -6.09807 LUMO: 0.16871 factor:1 | 1 (-0.42967) | -1 | -1 |
| G: -5312.42844 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.11708 HOMO: -6.72393 LUMO: 0.27211 factor:1 | 1 (-0.32294) | -1 | -1 |
| G: -5312.42844 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.60969 HOMO: -6.40556 LUMO: -0.04354 factor:1 | 1 (-0.81555) | -1 | -1 |
| G: -5312.42844 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.16239 HOMO: -6.56883 LUMO: 0.22041 factor:1 | 1 (-0.36825) | -1 | -1 |
| G: -5312.42844 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.27962 HOMO: -7.22462 LUMO: 0.15783 factor:1 | 1 (-0.48548) | 1 | 1 |
| G: -5312.42844 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.36359 HOMO: -6.83550 LUMO: 0.19320 factor:1 | 1 (-0.56945) | -1 | -1 |
| G: -5312.42844 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11578.11743 HOMO: -7.26816 LUMO: -0.07619 factor:1 | 1 (-1.32329) | 1 | -1 |
| G: -5312.42844 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11578.01816 HOMO: -7.13483 LUMO: 0.33198 factor:1 | 1 (-1.22402) | 1 | 1 |
| G: -5312.42844 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11578.34641 HOMO: -6.58243 LUMO: -0.26395 factor:1 | 1 (-1.55227) | -1 | -1 |
| G: -5312.42844 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.81614 HOMO: -7.38517 LUMO: 0.17143 factor:1 | 1 (-1.02201) | 1 | 1 |
| G: -5312.42844 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11578.72579 HOMO: -6.80013 LUMO: 0.25851 factor:1 | 1 (-1.93165) | -1 | -1 |
| G: -5312.42844 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11578.20976 HOMO: -6.96611 LUMO: 0.11429 factor:1 | 1 (-1.41562) | -1 | -1 |
| G: -5312.42844 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11578.40336 HOMO: -6.51713 LUMO: -1.14560 factor:1 | 1 (-1.60923) | -1 | -1 |
| G: -5312.42844 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11578.39887 HOMO: -7.15387 LUMO: -0.35647 factor:1 | 1 (-1.60474) | 1 | 1 |
| G: -5312.42844 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11578.77831 HOMO: -5.26540 LUMO: 1.26805 factor:1 | 1 (-1.98417) | -1 | -1 |
| G: -5312.42844 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11578.21773 HOMO: -6.76475 LUMO: -0.16327 factor:1 | 1 (-1.42359) | -1 | -1 |
| G: -5312.42844 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11578.53074 HOMO: -6.55250 LUMO: -0.71838 factor:1 | 1 (-1.73660) | -1 | -1 |
| G: -5312.42844 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11579.08836 HOMO: -6.76203 LUMO: -1.08301 factor:1 | 1 (-2.29422) | -1 | -1 |
| G: -5312.42844 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11578.82120 HOMO: -7.14027 LUMO: -0.01633 factor:1 | 1 (-2.02706) | 1 | 1 |
| G: -5312.42844 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11578.27542 HOMO: -6.94979 LUMO: -0.93879 factor:1 | 1 (-1.48128) | -1 | -1 |
| G: -5312.42844 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11578.38184 HOMO: -6.74842 LUMO: 0.31293 factor:1 | 1 (-1.58770) | -1 | -1 |
| G: -5312.42844 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11578.16682 HOMO: -6.43821 LUMO: 0.05987 factor:1 | 1 (-1.37268) | -1 | -1 |
| G: -5312.42844 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11579.02120 HOMO: -6.60420 LUMO: 0.22585 factor:1 | 1 (-2.22706) | -1 | -1 |
| G: -5312.42844 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11578.83913 HOMO: -6.43821 LUMO: 0.05987 factor:1 | 1 (-2.04499) | -1 | -1 |
| G: -5312.42844 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11578.03351 HOMO: -6.34570 LUMO: 1.43948 factor:1 | 1 (-1.23937) | -1 | -1 |
| G: -5312.42844 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11578.23299 HOMO: -6.03004 LUMO: 1.21363 factor:1 | 1 (-1.43886) | -1 | -1 |
| G: -5312.42844 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.84477 HOMO: -6.68040 LUMO: -0.92247 factor:1 | 1 (-1.05063) | -1 | -1 |
| G: -5312.42844 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.79947 HOMO: -6.92530 LUMO: -0.31293 factor:1 | 1 (-0.00533) | -1 | -1 |
| G: -5312.42844 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.84769 HOMO: -6.94979 LUMO: -0.19864 factor:1 | 1 (-0.05355) | -1 | -1 |
| G: -5312.42844 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.86249 HOMO: -6.80829 LUMO: -0.30477 factor:1 | 1 (-0.06836) | -1 | -1 |
| G: -5312.42844 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.62652 HOMO: -7.22734 LUMO: -1.02859 factor:1 | -1 (0.16762) | 1 | 1 |
| G: -5312.42844 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.73604 HOMO: -6.93890 LUMO: -0.72382 factor:1 | -1 (0.05810) | -1 | -1 |
| G: -5312.42844 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.66398 HOMO: -7.27088 LUMO: -0.78097 factor:1 | 1 (-0.86984) | 1 | 1 |
| G: -5312.42844 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.89965 HOMO: -7.29809 LUMO: -0.97145 factor:1 | 1 (-1.10552) | 1 | 1 |
| G: -5312.42844 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.91835 HOMO: -7.18925 LUMO: -0.94696 factor:1 | 1 (-1.12421) | 1 | 1 |
| G: -5312.42844 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.59715 HOMO: -7.33891 LUMO: -0.96873 factor:1 | 1 (-0.80301) | 1 | 1 |
| G: -5312.42844 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.86385 HOMO: -7.36068 LUMO: -0.28028 factor:1 | 1 (-0.06972) | 1 | 1 |
| G: -5312.42844 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.86021 HOMO: -7.10761 LUMO: -1.14832 factor:1 | 1 (-0.06607) | 1 | 1 |
| G: -5312.42844 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.02035 HOMO: -6.94707 LUMO: -0.65307 factor:1 | 1 (-0.22621) | -1 | -1 |
| G: -5312.42844 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.22378 HOMO: -6.91713 LUMO: -1.81228 factor:1 | 1 (-0.42964) | -1 | -1 |
| G: -5312.42844 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.09305 HOMO: -6.78652 LUMO: -2.01636 factor:1 | 1 (-0.29892) | -1 | -1 |
| G: -5312.42844 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.71770 HOMO: -6.52801 LUMO: -1.17553 factor:1 | -1 (0.07644) | -1 | -1 |
| G: -5312.42844 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.80674 HOMO: -7.54844 LUMO: -1.18642 factor:1 | 1 (-0.01260) | 1 | -1 |
| G: -5312.42844 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.72845 HOMO: -7.52939 LUMO: -1.23812 factor:1 | -1 (0.06569) | 1 | -1 |
| G: -5312.42844 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.05586 HOMO: -7.94572 LUMO: -0.81634 factor:1 | 1 (-0.26172) | 1 | 1 |
| G: -5312.42844 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.82402 HOMO: -7.55932 LUMO: -0.86260 factor:1 | 1 (-0.02988) | 1 | 1 |
| G: -5312.42844 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.98347 HOMO: -7.72259 LUMO: -1.39050 factor:1 | 1 (-0.18934) | 1 | -1 |
| G: -5312.42844 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.21616 HOMO: -7.11850 LUMO: -1.01498 factor:1 | 1 (-0.42202) | 1 | -1 |
| G: -5312.42844 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.55585 HOMO: -7.09673 LUMO: -1.00954 factor:1 | -1 (0.23829) | 1 | -1 |
| G: -5312.42844 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.69454 HOMO: -6.06270 LUMO: 0.16327 factor:1 | -1 (0.09959) | -1 | -1 |
| G: -5312.42844 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.89047 HOMO: -5.71167 LUMO: 0.70477 factor:1 | 1 (-0.09633) | -1 | -1 |
| G: -5312.42844 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.68799 HOMO: -5.38241 LUMO: 0.86260 factor:1 | -1 (0.10615) | -1 | -1 |
| G: -5312.42844 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.13257 HOMO: -5.67357 LUMO: 1.27621 factor:1 | 1 (-0.33843) | -1 | -1 |
| G: -5312.42844 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.19061 HOMO: -7.56204 LUMO: -0.68573 factor:1 | 1 (-0.39647) | 1 | 1 |
| G: -5312.42844 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.92418 HOMO: -5.57833 LUMO: 1.13199 factor:1 | 1 (-0.13004) | -1 | -1 |
| G: -5312.42844 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.76323 HOMO: -7.58653 LUMO: -0.66124 factor:1 | -1 (0.03091) | 1 | 1 |
| G: -5312.42844 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.61057 HOMO: -7.91851 LUMO: -1.10206 factor:1 | -1 (0.18357) | 1 | -1 |
| G: -5312.42844 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11578.08398 HOMO: -6.48992 LUMO: -1.00138 factor:1 | 1 (-1.28985) | -1 | -1 |
| G: -5312.42844 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11579.01891 HOMO: -7.09673 LUMO: -0.45171 factor:1 | 1 (-2.22478) | 1 | 1 |
| G: -5312.42844 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11578.31131 HOMO: -6.63686 LUMO: 0.09252 factor:1 | 1 (-1.51717) | -1 | -1 |
| G: -5312.42844 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11578.02292 HOMO: -6.84366 LUMO: -0.14422 factor:1 | 1 (-1.22878) | -1 | -1 |
| G: -5312.42844 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.78320 HOMO: -6.93074 LUMO: 0.04354 factor:1 | -1 (0.01094) | -1 | -1 |
| G: -5312.42844 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.75087 HOMO: -6.90353 LUMO: -0.19864 factor:1 | -1 (0.04327) | -1 | -1 |
| G: -5312.42844 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.07145 HOMO: -6.59876 LUMO: -0.10068 factor:1 | 1 (-0.27731) | -1 | -1 |
| G: -5312.42844 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.99123 HOMO: -6.74570 LUMO: -0.44627 factor:1 | 1 (-0.19709) | -1 | -1 |
| G: -5312.42844 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.66284 HOMO: -6.60148 LUMO: -0.61770 factor:1 | -1 (0.13129) | -1 | -1 |
| G: -5312.42844 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.77301 HOMO: -6.55794 LUMO: -1.06941 factor:1 | 1 (-0.97888) | -1 | -1 |
| G: -5312.42844 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11578.40494 HOMO: -7.12666 LUMO: -0.11973 factor:1 | 1 (-1.61081) | 1 | 1 |
| G: -5312.42844 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.74382 HOMO: -7.21646 LUMO: -0.50069 factor:1 | 1 (-0.94968) | 1 | 1 |
| G: -5312.42844 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.99171 HOMO: -7.27632 LUMO: -1.00682 factor:1 | 1 (-1.19757) | 1 | -1 |
| G: -5312.42844 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.68654 HOMO: -6.74298 LUMO: 0.04354 factor:1 | 1 (-0.89240) | -1 | -1 |
| G: -5312.42844 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.69530 HOMO: -6.37291 LUMO: 0.14150 factor:1 | 1 (-0.90116) | -1 | -1 |
| G: -5312.42844 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.91348 HOMO: -5.61371 LUMO: 1.28438 factor:1 | 1 (-1.11934) | -1 | -1 |
| G: -5312.42844 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.92741 HOMO: -5.52119 LUMO: 0.99866 factor:1 | 1 (-1.13327) | -1 | -1 |
| G: -5312.42844 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.50670 HOMO: -6.51985 LUMO: -0.10885 factor:1 | 1 (-0.71256) | -1 | -1 |
| G: -5312.42844 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11578.06241 HOMO: -5.61371 LUMO: 0.77280 factor:1 | 1 (-1.26827) | -1 | -1 |
| G: -5312.42844 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.97402 HOMO: -5.58922 LUMO: 0.24490 factor:1 | 1 (-1.17989) | -1 | -1 |
| G: -5312.42844 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11578.26331 HOMO: -6.32665 LUMO: -0.57144 factor:1 | 1 (-1.46917) | -1 | -1 |
| G: -5312.42844 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.73931 HOMO: -6.29127 LUMO: -0.93607 factor:1 | -1 (0.05483) | -1 | -1 |
| G: -5312.42844 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.83144 HOMO: -5.49670 LUMO: 0.27211 factor:1 | 1 (-0.03731) | -1 | -1 |
| G: -5312.42844 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.57781 HOMO: -5.68990 LUMO: 0.24218 factor:1 | -1 (0.21633) | -1 | -1 |
| G: -5312.42844 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.89564 HOMO: -5.68174 LUMO: 0.69933 factor:1 | 1 (-0.10150) | -1 | -1 |
| G: -5312.42844 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.04369 HOMO: -5.28173 LUMO: 1.00954 factor:1 | 1 (-0.24956) | -1 | -1 |
| G: -5312.42844 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.61098 HOMO: -5.94025 LUMO: 0.73471 factor:1 | -1 (0.18316) | -1 | -1 |
| G: -5312.42844 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11578.45460 HOMO: -5.65725 LUMO: 1.28710 factor:1 | 1 (-1.66047) | -1 | -1 |
| G: -5312.42844 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.63078 HOMO: -5.41507 LUMO: 0.87076 factor:1 | 1 (-0.83664) | -1 | -1 |
| G: -5312.42844 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.76730 HOMO: -5.96474 LUMO: 0.29660 factor:1 | 1 (-0.97316) | -1 | -1 |
| G: -5312.42844 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.91810 HOMO: -7.00421 LUMO: 0.08708 factor:1 | 1 (-1.12397) | -1 | -1 |
| G: -5312.42844 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11578.14880 HOMO: -5.40418 LUMO: 0.90070 factor:1 | 1 (-1.35466) | -1 | -1 |
| G: -5312.42844 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11578.33079 HOMO: -7.00421 LUMO: -0.30477 factor:1 | 1 (-1.53665) | -1 | -1 |
| G: -5312.42844 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11578.37721 HOMO: -5.85861 LUMO: 0.74015 factor:1 | 1 (-1.58308) | -1 | -1 |
| G: -5312.42844 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.91239 HOMO: -5.71439 LUMO: 0.26395 factor:1 | 1 (-1.11825) | -1 | -1 |
| G: -5312.42844 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.64634 HOMO: -7.13755 LUMO: -0.78369 factor:1 | 1 (-0.85221) | 1 | -1 |
| G: -5312.42844 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.88866 HOMO: -7.31442 LUMO: -0.98233 factor:1 | 1 (-1.09452) | 1 | -1 |
| G: -5312.42844 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.93949 HOMO: -7.25728 LUMO: -1.00410 factor:1 | 1 (-1.14535) | 1 | -1 |
| G: -5312.42844 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.66830 HOMO: -7.48585 LUMO: -0.83811 factor:1 | 1 (-0.87417) | 1 | -1 |
| G: -5312.42844 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11578.10924 HOMO: -7.24911 LUMO: -0.77280 factor:1 | 1 (-1.31510) | 1 | -1 |
| G: -5312.42844 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11578.33316 HOMO: -7.55116 LUMO: -1.19730 factor:1 | 1 (-1.53902) | 1 | -1 |
| G: -5312.42844 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11578.24845 HOMO: -5.76881 LUMO: 0.28028 factor:1 | 1 (-1.45431) | -1 | -1 |
| G: -5312.42844 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11578.01057 HOMO: -5.77153 LUMO: -0.26939 factor:1 | 1 (-1.21643) | -1 | -1 |
| G: -5312.42844 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.89724 HOMO: -5.82868 LUMO: 0.36735 factor:1 | 1 (-0.10310) | -1 | -1 |
| G: -5312.42844 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.74214 HOMO: -5.83140 LUMO: -0.17960 factor:1 | -1 (0.05200) | -1 | -1 |
| G: -5312.42844 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.87251 HOMO: -6.28855 LUMO: 0.01088 factor:1 | 1 (-0.07837) | -1 | -1 |
| G: -5312.42844 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.94647 HOMO: -6.31576 LUMO: 0.25307 factor:1 | 1 (-0.15233) | -1 | -1 |
| G: -5312.42844 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.93477 HOMO: -7.06408 LUMO: -2.76196 factor:1 | 1 (-0.14063) | -1 | -1 |
| G: -5312.42844 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.00935 HOMO: -5.95657 LUMO: 0.37552 factor:1 | 1 (-0.21521) | -1 | -1 |
| G: -5312.42844 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.60404 HOMO: -6.61781 LUMO: 0.02721 factor:1 | -1 (0.19010) | -1 | -1 |
| G: -5312.42844 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.82151 HOMO: -6.26678 LUMO: -0.66668 factor:1 | 1 (-0.02737) | -1 | -1 |
| G: -5312.42844 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.69709 HOMO: -6.00011 LUMO: -0.13334 factor:1 | 1 (-0.90296) | -1 | -1 |
| G: -5312.42844 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11578.51531 HOMO: -5.60555 LUMO: 0.67484 factor:1 | 1 (-1.72117) | -1 | -1 |
| G: -5312.42844 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.89508 HOMO: -5.79875 LUMO: 0.99049 factor:1 | 1 (-1.10095) | -1 | -1 |
| G: -5312.42844 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.93759 HOMO: -5.97834 LUMO: 0.48436 factor:1 | 1 (-1.14345) | -1 | -1 |
| G: -5312.42844 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.63894 HOMO: -5.82868 LUMO: 0.91974 factor:1 | 1 (-0.84480) | -1 | -1 |
| G: -5312.42844 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.71595 HOMO: -5.86677 LUMO: 0.99594 factor:1 | 1 (-0.92181) | -1 | -1 |
| G: -5312.42844 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.60123 HOMO: -5.70079 LUMO: 0.48980 factor:1 | 1 (-0.80709) | -1 | -1 |
| G: -5312.42844 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.75565 HOMO: -7.39605 LUMO: -1.02315 factor:1 | 1 (-0.96151) | 1 | -1 |
| G: -5312.42844 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.65124 HOMO: -7.22734 LUMO: -1.12927 factor:1 | 1 (-0.85710) | 1 | -1 |
| G: -5312.42844 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.98387 HOMO: -7.58926 LUMO: -0.65035 factor:1 | 1 (-1.18974) | 1 | 1 |
| G: -5312.42844 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.89887 HOMO: -7.43959 LUMO: -0.75648 factor:1 | 1 (-0.10474) | 1 | 1 |
| G: -5312.42844 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.09417 HOMO: -7.55388 LUMO: -1.15104 factor:1 | 1 (-0.30003) | 1 | -1 |
| G: -5312.42844 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.98334 HOMO: -6.74570 LUMO: -2.85447 factor:1 | 1 (-0.18920) | -1 | -1 |
| G: -5312.42844 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.03205 HOMO: -7.35524 LUMO: -1.25444 factor:1 | 1 (-0.23791) | 1 | 1 |
| G: -5312.42844 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.01289 HOMO: -6.81645 LUMO: -1.20819 factor:1 | 1 (-0.21875) | -1 | -1 |
| G: -5312.42844 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.98630 HOMO: -6.99605 LUMO: -1.62996 factor:1 | 1 (-0.19217) | -1 | -1 |
| G: -5312.42844 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.23306 HOMO: -6.88992 LUMO: -0.47620 factor:1 | 1 (-0.43892) | -1 | -1 |
| G: -5312.42844 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.17899 HOMO: -7.22190 LUMO: -0.01905 factor:1 | 1 (-0.38485) | 1 | 1 |
| G: -5312.42844 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.77172 HOMO: -6.77836 LUMO: -0.82995 factor:1 | -1 (0.02242) | -1 | -1 |
| G: -5312.42844 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.86576 HOMO: -6.48447 LUMO: -0.95512 factor:1 | 1 (-0.07162) | -1 | -1 |
| G: -5312.42844 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.77947 HOMO: -7.81239 LUMO: 1.22179 factor:1 | -1 (0.01467) | 1 | 1 |
| G: -5312.42844 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.99703 HOMO: -7.36612 LUMO: 0.19320 factor:1 | 1 (-0.20289) | 1 | 1 |
| G: -5312.42844 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.72744 HOMO: -7.24095 LUMO: 0.33470 factor:1 | -1 (0.06670) | 1 | 1 |
| G: -5312.42844 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.03088 HOMO: -7.15932 LUMO: -2.24222 factor:1 | 1 (-0.23674) | -1 | -1 |
| G: -5312.42844 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.98870 HOMO: -6.88992 LUMO: -2.69937 factor:1 | 1 (-0.19456) | -1 | -1 |
| G: -5312.42844 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.95659 HOMO: -6.97428 LUMO: -0.98233 factor:1 | 1 (-0.16245) | -1 | -1 |
| G: -5312.42844 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.06827 HOMO: -7.17564 LUMO: -0.93879 factor:1 | 1 (-0.27413) | 1 | 1 |
| G: -5312.42844 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.91120 HOMO: -6.81645 LUMO: -1.14288 factor:1 | 1 (-0.11706) | -1 | -1 |
| G: -5312.42844 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.25461 HOMO: -6.83006 LUMO: -0.63403 factor:1 | 1 (-0.46047) | -1 | -1 |
| G: -5312.42844 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.89262 HOMO: -7.17292 LUMO: -1.07213 factor:1 | 1 (-0.09848) | 1 | 1 |
| G: -5312.42844 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.63503 HOMO: -7.53755 LUMO: 0.15510 factor:1 | -1 (0.15910) | 1 | 1 |
| G: -5312.42844 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.90687 HOMO: -6.50080 LUMO: -0.51702 factor:1 | 1 (-0.11274) | -1 | -1 |
| G: -5312.42844 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.69424 HOMO: -6.72665 LUMO: -0.80001 factor:1 | -1 (0.09989) | -1 | -1 |
| G: -5312.42844 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.97615 HOMO: -6.72665 LUMO: 1.68711 factor:1 | 1 (-0.18202) | -1 | -1 |
| G: -5312.42844 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.05997 HOMO: -7.11850 LUMO: -0.75103 factor:1 | 1 (-0.26583) | 1 | 1 |
| G: -5312.42844 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.75988 HOMO: -6.87087 LUMO: -0.85988 factor:1 | -1 (0.03426) | -1 | -1 |
| G: -5312.42844 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.98138 HOMO: -7.08857 LUMO: -0.89798 factor:1 | 1 (-0.18724) | 1 | 1 |
| G: -5312.42844 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.89180 HOMO: -6.71305 LUMO: -0.85444 factor:1 | 1 (-0.09766) | -1 | -1 |
| G: -5312.42844 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.85800 HOMO: -6.59332 LUMO: -0.60137 factor:1 | 1 (-0.06387) | -1 | -1 |
| G: -5312.42844 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.76976 HOMO: -7.28993 LUMO: 0.03265 factor:1 | -1 (0.02438) | 1 | 1 |
| G: -5312.42844 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.49481 HOMO: -7.32258 LUMO: 0.13878 factor:1 | -1 (0.29933) | 1 | 1 |
| G: -5312.42844 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.62687 HOMO: -7.28993 LUMO: 0.11429 factor:1 | -1 (0.16727) | 1 | 1 |
| G: -5312.42844 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.54031 HOMO: -6.86271 LUMO: -1.03947 factor:1 | -1 (0.25383) | -1 | -1 |
| G: -5312.42844 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.89172 HOMO: -6.55794 LUMO: -0.84900 factor:1 | 1 (-0.09758) | -1 | -1 |
| G: -5312.42844 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.98587 HOMO: -7.03686 LUMO: 0.11429 factor:1 | 1 (-0.19173) | -1 | -1 |
| G: -5312.42844 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.88747 HOMO: -7.06952 LUMO: -0.96056 factor:1 | 1 (-0.09334) | 1 | 1 |
| G: -5312.42844 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.07205 HOMO: -6.90897 LUMO: -0.99866 factor:1 | 1 (-0.27791) | -1 | -1 |
| G: -5312.42844 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.73454 HOMO: -7.00693 LUMO: -0.83539 factor:1 | -1 (0.05959) | -1 | -1 |
| G: -5312.42844 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.13338 HOMO: -6.74298 LUMO: -0.85172 factor:1 | 1 (-0.33924) | -1 | -1 |
| G: -5312.42844 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.00307 HOMO: -6.83822 LUMO: -1.07213 factor:1 | 1 (-0.20893) | -1 | -1 |
| G: -5312.42844 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.07828 HOMO: -7.21918 LUMO: -1.55377 factor:1 | 1 (-0.28414) | 1 | 1 |
| G: -5312.42844 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.34928 HOMO: -6.84094 LUMO: -1.09934 factor:1 | 1 (-0.55514) | -1 | -1 |
| G: -5312.42844 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.16389 HOMO: -7.09129 LUMO: -0.85988 factor:1 | 1 (-0.36975) | 1 | 1 |
| G: -5312.42844 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.98269 HOMO: -6.57971 LUMO: -2.27215 factor:1 | 1 (-0.18855) | -1 | -1 |
| G: -5312.42844 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.92598 HOMO: -6.81373 LUMO: -1.86942 factor:1 | 1 (-0.13184) | -1 | -1 |
| G: -5312.42844 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.99847 HOMO: -6.59060 LUMO: -2.30480 factor:1 | 1 (-0.20433) | -1 | -1 |
| G: -5312.42844 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.17564 HOMO: -6.72938 LUMO: -1.23540 factor:1 | 1 (-0.38150) | -1 | -1 |
| G: -5312.42844 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.10756 HOMO: -6.94707 LUMO: -2.62318 factor:1 | 1 (-0.31342) | -1 | -1 |
| G: -5312.42844 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.14965 HOMO: -7.28177 LUMO: -0.09796 factor:1 | 1 (-0.35552) | 1 | 1 |
| G: -5312.42844 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.28718 HOMO: -6.80013 LUMO: -0.79729 factor:1 | 1 (-0.49304) | -1 | -1 |
| G: -5312.42844 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.83634 HOMO: -7.26544 LUMO: 0.12789 factor:1 | 1 (-0.04220) | 1 | 1 |
| G: -5312.42844 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.87689 HOMO: -6.51713 LUMO: -0.49253 factor:1 | 1 (-0.08275) | -1 | -1 |
| G: -5312.42844 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.76159 HOMO: -6.68856 LUMO: -0.77280 factor:1 | -1 (0.03254) | -1 | -1 |
| G: -5312.42844 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.96622 HOMO: -6.41100 LUMO: -0.70750 factor:1 | 1 (-0.17208) | -1 | -1 |
| G: -5312.42844 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.91131 HOMO: -7.56204 LUMO: 0.22041 factor:1 | 1 (-0.11717) | 1 | 1 |
| G: -5312.42844 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.75297 HOMO: -6.68312 LUMO: 1.30343 factor:1 | -1 (0.04117) | -1 | -1 |
| G: -5312.42844 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.09314 HOMO: -7.24367 LUMO: 0.17415 factor:1 | 1 (-0.29900) | 1 | 1 |
| G: -5312.42844 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.01210 HOMO: -7.52395 LUMO: 1.16737 factor:1 | 1 (-0.21796) | 1 | 1 |
| G: -5312.42844 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.00995 HOMO: -6.89264 LUMO: 0.23130 factor:1 | 1 (-0.21581) | -1 | -1 |
| G: -5312.42844 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.68614 HOMO: -7.21102 LUMO: 0.19048 factor:1 | -1 (0.10800) | 1 | 1 |
| G: -5312.42844 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.64532 HOMO: -7.08312 LUMO: 0.25034 factor:1 | -1 (0.14882) | 1 | 1 |
| G: -5312.42844 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.46450 HOMO: -6.49536 LUMO: -0.65852 factor:1 | -1 (0.32964) | -1 | -1 |
| G: -5312.42844 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.57027 HOMO: -6.85455 LUMO: 0.13606 factor:1 | -1 (0.22387) | -1 | -1 |
| G: -5312.42844 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.93199 HOMO: -7.10217 LUMO: 0.35919 factor:1 | 1 (-0.13785) | 1 | 1 |
| G: -5312.42844 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.86516 HOMO: -7.77429 LUMO: 1.19186 factor:1 | 1 (-0.07102) | 1 | 1 |
| G: -5312.42844 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.87806 HOMO: -6.57427 LUMO: -0.50069 factor:1 | 1 (-0.08392) | -1 | -1 |
| G: -5312.42844 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.01920 HOMO: -7.36340 LUMO: 0.10068 factor:1 | 1 (-0.22507) | 1 | 1 |
| G: -5312.42844 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.99382 HOMO: -7.28177 LUMO: 0.15238 factor:1 | 1 (-0.19968) | 1 | 1 |
| G: -5312.42844 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.21148 HOMO: -6.86543 LUMO: -0.84355 factor:1 | 1 (-0.41734) | -1 | -1 |
| G: -5312.42844 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.05012 HOMO: -6.55794 LUMO: 1.39594 factor:1 | 1 (-0.25598) | -1 | -1 |
| G: -5312.42844 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.05969 HOMO: -6.26134 LUMO: 1.53744 factor:1 | 1 (-0.26556) | -1 | -1 |
| G: -5312.42844 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.91713 HOMO: -5.97562 LUMO: 1.42316 factor:1 | 1 (-0.12300) | -1 | -1 |
| G: -5312.42844 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.74649 HOMO: -6.65046 LUMO: 1.44492 factor:1 | -1 (0.04765) | -1 | -1 |
| G: -5312.42844 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.71291 HOMO: -6.92258 LUMO: 0.17415 factor:1 | -1 (0.08123) | -1 | -1 |
| G: -5312.42844 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.62253 HOMO: -7.40966 LUMO: 0.19592 factor:1 | 1 (-0.82840) | 1 | 1 |
| G: -5312.42844 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.46533 HOMO: -7.17564 LUMO: 0.16871 factor:1 | 1 (-0.67120) | 1 | 1 |
| G: -5312.42844 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.58476 HOMO: -7.46953 LUMO: 0.22313 factor:1 | 1 (-0.79063) | 1 | 1 |
| G: -5312.42844 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.75299 HOMO: -6.13345 LUMO: 1.85854 factor:1 | 1 (-0.95885) | -1 | -1 |
| G: -5312.42844 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.85318 HOMO: -6.99333 LUMO: -1.65717 factor:1 | 1 (-1.05904) | -1 | -1 |
| G: -5312.42844 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.64346 HOMO: -6.93074 LUMO: -1.79323 factor:1 | 1 (-0.84932) | -1 | -1 |
| G: -5312.42844 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.48506 HOMO: -6.87904 LUMO: -1.79323 factor:1 | 1 (-0.69092) | -1 | -1 |
| G: -5312.42844 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.33309 HOMO: -6.84094 LUMO: 0.66940 factor:1 | 1 (-0.53895) | -1 | -1 |
| G: -5312.42844 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.73184 HOMO: -7.13210 LUMO: -1.17553 factor:1 | 1 (-0.93770) | 1 | 1 |
| G: -5312.42844 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11578.19977 HOMO: -6.52801 LUMO: -2.23678 factor:1 | 1 (-1.40563) | -1 | -1 |
| G: -5312.42844 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11578.08622 HOMO: -6.81917 LUMO: -1.86398 factor:1 | 1 (-1.29208) | -1 | -1 |
| G: -5312.42844 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11578.23781 HOMO: -7.30626 LUMO: -1.66806 factor:1 | 1 (-1.44367) | 1 | 1 |
| G: -5312.42844 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11578.80296 HOMO: -6.98516 LUMO: -1.40683 factor:1 | 1 (-2.00883) | -1 | -1 |
| G: -5312.42844 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11579.10817 HOMO: -6.95523 LUMO: -0.97145 factor:1 | 1 (-2.31403) | -1 | -1 |
| G: -5312.42844 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11578.32276 HOMO: -6.83278 LUMO: -2.68848 factor:1 | 1 (-1.52863) | -1 | -1 |
| G: -5312.42844 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.77533 HOMO: -7.25456 LUMO: -2.97420 factor:1 | 1 (-0.98119) | -1 | -1 |
| G: -5312.42844 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.98591 HOMO: -6.80557 LUMO: -2.65039 factor:1 | 1 (-1.19178) | -1 | -1 |
| G: -5312.42844 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.87840 HOMO: -7.10489 LUMO: 0.77008 factor:1 | 1 (-1.08426) | 1 | -1 |
| G: -5312.42844 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.97277 HOMO: -7.28993 LUMO: -1.06124 factor:1 | 1 (-1.17863) | 1 | 1 |
| G: -5312.42844 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.69840 HOMO: -7.11578 LUMO: -1.10206 factor:1 | 1 (-0.90426) | 1 | 1 |
| G: -5312.42844 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.94856 HOMO: -6.91713 LUMO: -1.36329 factor:1 | 1 (-0.15442) | -1 | -1 |
| G: -5312.42844 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.87166 HOMO: -7.07224 LUMO: 0.51974 factor:1 | 1 (-0.07753) | 1 | 1 |
| G: -5312.42844 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.90965 HOMO: -7.22734 LUMO: -0.93335 factor:1 | 1 (-0.11551) | 1 | 1 |
| G: -5312.42844 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.00655 HOMO: -7.19469 LUMO: -0.96600 factor:1 | 1 (-0.21241) | 1 | 1 |
| G: -5312.42844 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.11714 HOMO: -6.93890 LUMO: -0.66940 factor:1 | 1 (-0.32300) | -1 | -1 |
| G: -5312.42844 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.12220 HOMO: -7.09673 LUMO: -1.05852 factor:1 | 1 (-0.32806) | 1 | 1 |
| G: -5312.42844 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.85648 HOMO: -7.19197 LUMO: -2.26943 factor:1 | 1 (-0.06234) | -1 | -1 |
| G: -5312.42844 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.81740 HOMO: -6.90081 LUMO: -2.64767 factor:1 | 1 (-0.02327) | -1 | -1 |
| G: -5312.42844 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.81618 HOMO: -6.93890 LUMO: -2.65039 factor:1 | 1 (-0.02204) | -1 | -1 |
| G: -5312.42844 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.95885 HOMO: -6.80013 LUMO: -2.54154 factor:1 | 1 (-0.16471) | -1 | -1 |
| G: -5312.42844 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.83052 HOMO: -6.68040 LUMO: -0.89798 factor:1 | 1 (-0.03638) | -1 | -1 |
| G: -5312.42844 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.01050 HOMO: -7.01782 LUMO: -1.09662 factor:1 | 1 (-0.21636) | -1 | -1 |
| G: -5312.42844 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.80295 HOMO: -6.58516 LUMO: -0.83539 factor:1 | 1 (-0.00882) | -1 | -1 |
| G: -5312.42844 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.01471 HOMO: -7.46953 LUMO: 0.06259 factor:1 | 1 (-0.22058) | 1 | 1 |
| G: -5312.42844 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.19855 HOMO: -6.96884 LUMO: -0.99866 factor:1 | 1 (-0.40442) | -1 | -1 |
| G: -5312.42844 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.72736 HOMO: -7.29809 LUMO: -0.19320 factor:1 | -1 (0.06678) | 1 | 1 |
| G: -5312.42844 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.88973 HOMO: -6.86271 LUMO: 0.04082 factor:1 | 1 (-0.09559) | -1 | -1 |
| G: -5312.42844 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.88704 HOMO: -6.36746 LUMO: -1.02587 factor:1 | 1 (-0.09290) | -1 | -1 |
| G: -5312.42844 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.73245 HOMO: -7.15659 LUMO: -1.25989 factor:1 | -1 (0.06169) | 1 | 1 |
| G: -5312.42844 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.97768 HOMO: -6.69128 LUMO: -0.59865 factor:1 | 1 (-0.18354) | -1 | -1 |
| G: -5312.42844 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.81076 HOMO: -7.09129 LUMO: -1.08573 factor:1 | 1 (-0.01663) | 1 | 1 |
| G: -5312.42844 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.05297 HOMO: -6.64502 LUMO: -0.66396 factor:1 | 1 (-0.25883) | -1 | -1 |
| G: -5312.42844 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.90119 HOMO: -6.93346 LUMO: -0.87349 factor:1 | 1 (-0.10705) | -1 | -1 |
| G: -5312.42844 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.74421 HOMO: -6.77019 LUMO: -0.87349 factor:1 | -1 (0.04993) | -1 | -1 |
| G: -5312.42844 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.64317 HOMO: -6.59060 LUMO: -0.82995 factor:1 | -1 (0.15097) | -1 | -1 |
| G: -5312.42844 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.00709 HOMO: -7.17564 LUMO: -1.08846 factor:1 | 1 (-0.21296) | 1 | 1 |
| G: -5312.42844 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11578.18804 HOMO: -7.27088 LUMO: -1.18642 factor:1 | 1 (-1.39390) | 1 | 1 |
| G: -5312.42844 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11578.94767 HOMO: -7.06680 LUMO: -1.13199 factor:1 | 1 (-2.15354) | 1 | 1 |
| G: -5312.42844 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11578.05460 HOMO: -7.21918 LUMO: -1.03947 factor:1 | 1 (-1.26046) | 1 | 1 |
| G: -5312.42844 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11578.37251 HOMO: -7.26000 LUMO: -0.11973 factor:1 | 1 (-1.57837) | 1 | 1 |
| G: -5312.42844 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11578.11675 HOMO: -6.77564 LUMO: 0.23402 factor:1 | 1 (-1.32261) | -1 | -1 |
| G: -5312.42844 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.80815 HOMO: -7.07224 LUMO: -0.75648 factor:1 | 1 (-0.01401) | 1 | 1 |
| G: -5312.42844 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.66565 HOMO: -7.45048 LUMO: 0.18232 factor:1 | -1 (0.12849) | 1 | 1 |
| G: -5312.42844 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.82271 HOMO: -7.48313 LUMO: 0.15238 factor:1 | 1 (-0.02857) | 1 | 1 |
| G: -5312.42844 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.76521 HOMO: -6.60692 LUMO: -0.50885 factor:1 | -1 (0.02893) | -1 | -1 |
| G: -5312.42844 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.98837 HOMO: -6.62869 LUMO: -0.60954 factor:1 | 1 (-0.19423) | -1 | -1 |
| G: -5312.42844 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.71746 HOMO: -7.40422 LUMO: -1.28982 factor:1 | -1 (0.07668) | 1 | 1 |
| G: -5312.42844 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.72151 HOMO: -6.75114 LUMO: -1.23268 factor:1 | -1 (0.07263) | -1 | -1 |
| G: -5312.42844 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.47764 HOMO: -6.84638 LUMO: -0.73199 factor:1 | -1 (0.31650) | -1 | -1 |
| G: -5312.42844 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.97221 HOMO: -6.79196 LUMO: -1.43676 factor:1 | 1 (-0.17807) | -1 | -1 |
| G: -5312.42844 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.79710 HOMO: -7.00965 LUMO: -1.37690 factor:1 | 1 (-1.00296) | -1 | -1 |
| G: -5312.42844 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11578.39194 HOMO: -6.97972 LUMO: -1.58098 factor:1 | 1 (-1.59780) | -1 | -1 |
| G: -5312.42844 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.66313 HOMO: -6.91169 LUMO: -1.48574 factor:1 | 1 (-0.86900) | -1 | -1 |
| G: -5312.42844 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.80635 HOMO: -6.90081 LUMO: -1.30343 factor:1 | 1 (-1.01221) | -1 | -1 |
| G: -5312.42844 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.96902 HOMO: -6.78652 LUMO: -1.51840 factor:1 | 1 (-1.17488) | -1 | -1 |
| G: -5312.42844 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.70898 HOMO: -6.84638 LUMO: -1.15104 factor:1 | 1 (-0.91485) | -1 | -1 |
| G: -5312.42844 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.65320 HOMO: -6.61237 LUMO: -0.89798 factor:1 | 1 (-0.85906) | -1 | -1 |
| G: -5312.42844 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.97879 HOMO: -7.16204 LUMO: -1.30070 factor:1 | 1 (-1.18465) | 1 | 1 |
| G: -5312.42844 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.60357 HOMO: -7.32803 LUMO: 0.14694 factor:1 | 1 (-0.80943) | 1 | 1 |
| G: -5312.42844 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.78003 HOMO: -6.99877 LUMO: -0.87621 factor:1 | 1 (-0.98590) | -1 | -1 |
| G: -5312.42844 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.99318 HOMO: -6.99877 LUMO: -0.97145 factor:1 | 1 (-1.19904) | -1 | -1 |
| G: -5312.42844 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.89133 HOMO: -7.08040 LUMO: -1.09662 factor:1 | 1 (-1.09719) | 1 | 1 |
| G: -5312.42844 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.64357 HOMO: -6.90897 LUMO: -1.14016 factor:1 | 1 (-0.84943) | -1 | -1 |
| G: -5312.42844 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.71337 HOMO: -6.68312 LUMO: -0.74831 factor:1 | 1 (-0.91923) | -1 | -1 |
| G: -5312.42844 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.56610 HOMO: -6.99061 LUMO: -0.86804 factor:1 | 1 (-0.77196) | -1 | -1 |
| G: -5312.42844 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11578.20581 HOMO: -7.10761 LUMO: -1.18642 factor:1 | 1 (-1.41167) | 1 | 1 |
| G: -5312.42844 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11578.78011 HOMO: -6.79196 LUMO: -0.71294 factor:1 | 1 (-1.98597) | -1 | -1 |
| G: -5312.42844 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11578.16317 HOMO: -6.86271 LUMO: -0.81362 factor:1 | 1 (-1.36903) | -1 | -1 |
| G: -5312.42844 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.93772 HOMO: -7.01510 LUMO: -0.99322 factor:1 | 1 (-1.14359) | -1 | -1 |
| G: -5312.42844 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.96855 HOMO: -6.88720 LUMO: -0.87893 factor:1 | 1 (-1.17442) | -1 | -1 |
| G: -5312.42844 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.74956 HOMO: -6.88448 LUMO: 0.22041 factor:1 | 1 (-0.95542) | -1 | -1 |
| G: -5312.42844 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.61415 HOMO: -7.55932 LUMO: 1.12111 factor:1 | 1 (-0.82002) | 1 | 1 |
| G: -5312.42844 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.65117 HOMO: -6.46815 LUMO: -0.86260 factor:1 | -1 (0.14297) | -1 | -1 |
| G: -5312.42844 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.87381 HOMO: -7.13755 LUMO: 0.23130 factor:1 | 1 (-0.07967) | 1 | 1 |
| G: -5312.42844 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.86274 HOMO: -6.78924 LUMO: 1.51023 factor:1 | 1 (-0.06860) | -1 | -1 |
| G: -5312.42844 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.77433 HOMO: -6.48992 LUMO: 1.74969 factor:1 | -1 (0.01981) | -1 | -1 |
| G: -5312.42844 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.75863 HOMO: -6.78380 LUMO: 1.81500 factor:1 | -1 (0.03551) | -1 | -1 |
| G: -5312.42844 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.69073 HOMO: -6.49536 LUMO: 1.70615 factor:1 | -1 (0.10340) | -1 | -1 |
| G: -5312.42844 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.88622 HOMO: -6.38651 LUMO: 1.44492 factor:1 | 1 (-0.09208) | -1 | -1 |
| G: -5312.42844 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.68766 HOMO: -6.83822 LUMO: 1.38234 factor:1 | -1 (0.10648) | -1 | -1 |
| G: -5312.42844 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.96815 HOMO: -6.01644 LUMO: 1.20274 factor:1 | 1 (-0.17402) | -1 | -1 |
| G: -5312.42844 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.72434 HOMO: -6.18243 LUMO: 1.77962 factor:1 | -1 (0.06980) | -1 | -1 |
| G: -5312.42844 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.81936 HOMO: -6.81917 LUMO: -1.01771 factor:1 | 1 (-0.02522) | -1 | -1 |
| G: -5312.42844 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.56866 HOMO: -6.61237 LUMO: -0.91702 factor:1 | -1 (0.22547) | -1 | -1 |
| G: -5312.42844 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.96481 HOMO: -6.84094 LUMO: -0.84900 factor:1 | 1 (-0.17067) | -1 | -1 |
| G: -5312.42844 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.69520 HOMO: -6.81917 LUMO: -1.01771 factor:1 | -1 (0.09894) | -1 | -1 |
| G: -5312.42844 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.60766 HOMO: -7.86953 LUMO: 1.16737 factor:1 | -1 (0.18648) | 1 | 1 |
| G: -5312.42844 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.55049 HOMO: -7.40694 LUMO: 0.11429 factor:1 | -1 (0.24365) | 1 | 1 |
| G: -5312.42844 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.70728 HOMO: -6.70489 LUMO: -0.65035 factor:1 | -1 (0.08686) | -1 | -1 |
| G: -5312.42844 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.79612 HOMO: -7.23279 LUMO: 0.33470 factor:1 | 1 (-0.00199) | 1 | 1 |
| G: -5312.42844 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11578.01846 HOMO: -7.17020 LUMO: 0.41361 factor:1 | 1 (-1.22432) | 1 | 1 |
| G: -5312.42844 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11579.11029 HOMO: -6.90353 LUMO: -0.90070 factor:1 | 1 (-2.31615) | -1 | -1 |
| G: -5312.42844 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11578.18981 HOMO: -7.39061 LUMO: 0.17687 factor:1 | 1 (-1.39567) | 1 | 1 |
| G: -5312.42844 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.64992 HOMO: -7.16748 LUMO: 0.42178 factor:1 | -1 (0.14422) | 1 | 1 |
| G: -5312.42844 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.78140 HOMO: -7.36884 LUMO: -1.11295 factor:1 | -1 (0.01273) | 1 | 1 |
| G: -5312.42844 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.79923 HOMO: -7.33347 LUMO: 0.33198 factor:1 | 1 (-0.00509) | 1 | 1 |
| G: -5312.42844 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.64826 HOMO: -7.31986 LUMO: -0.83539 factor:1 | -1 (0.14588) | 1 | 1 |
| G: -5312.42844 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.81841 HOMO: -7.31170 LUMO: 0.08708 factor:1 | 1 (-0.02427) | 1 | 1 |
| G: -5312.42844 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11578.35662 HOMO: -7.36884 LUMO: 0.38096 factor:1 | 1 (-1.56248) | 1 | 1 |
| G: -5312.42844 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.73696 HOMO: -6.99333 LUMO: 1.74153 factor:1 | 1 (-0.94282) | -1 | -1 |
| G: -5312.42844 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.65111 HOMO: -6.94435 LUMO: 1.74969 factor:1 | 1 (-0.85697) | -1 | -1 |
| G: -5312.42844 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.76719 HOMO: -7.02598 LUMO: 1.43404 factor:1 | 1 (-0.97305) | -1 | -1 |
| G: -5312.42844 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.73451 HOMO: -6.41100 LUMO: 1.62996 factor:1 | 1 (-0.94037) | -1 | -1 |
| G: -5312.42844 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.85348 HOMO: -6.57699 LUMO: 1.81228 factor:1 | 1 (-1.05934) | -1 | -1 |
| G: -5312.42844 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11578.54348 HOMO: -6.86543 LUMO: 1.49935 factor:1 | 1 (-1.74934) | -1 | -1 |
| G: -5312.42844 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.61078 HOMO: -6.91169 LUMO: -1.22451 factor:1 | 1 (-0.81664) | -1 | -1 |
| G: -5312.42844 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.94834 HOMO: -7.09945 LUMO: -1.23812 factor:1 | 1 (-0.15421) | 1 | 1 |
| G: -5312.42844 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.11657 HOMO: -7.48857 LUMO: 0.10340 factor:1 | 1 (-0.32243) | 1 | 1 |
| G: -5312.42844 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.05782 HOMO: -7.21918 LUMO: -0.06803 factor:1 | 1 (-0.26368) | 1 | 1 |
| G: -5312.42844 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.05474 HOMO: -6.34025 LUMO: -0.68845 factor:1 | 1 (-0.26060) | -1 | -1 |
| G: -5312.42844 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.01033 HOMO: -6.82734 LUMO: -0.77825 factor:1 | 1 (-0.21619) | -1 | -1 |
| G: -5312.42844 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.11205 HOMO: -6.92258 LUMO: -1.03675 factor:1 | 1 (-0.31791) | -1 | -1 |
| G: -5312.42844 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.89569 HOMO: -6.42461 LUMO: -0.95240 factor:1 | 1 (-0.10155) | -1 | -1 |
| G: -5312.42844 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.76061 HOMO: -6.96067 LUMO: -1.05036 factor:1 | -1 (0.03352) | -1 | -1 |
| G: -5312.42844 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.28996 HOMO: -7.23551 LUMO: 0.12245 factor:1 | 1 (-0.49582) | 1 | 1 |
| G: -5312.42844 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.12642 HOMO: -6.85183 LUMO: 0.16055 factor:1 | 1 (-0.33228) | -1 | -1 |
| G: -5312.42844 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.16683 HOMO: -6.46815 LUMO: -0.89253 factor:1 | 1 (-0.37269) | -1 | -1 |
| G: -5312.42844 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.12282 HOMO: -7.23823 LUMO: -0.06259 factor:1 | 1 (-0.32869) | 1 | 1 |
| G: -5312.42844 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.26968 HOMO: -6.76475 LUMO: -0.99049 factor:1 | 1 (-0.47555) | -1 | -1 |
| G: -5312.42844 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.27975 HOMO: -7.14843 LUMO: -0.88165 factor:1 | 1 (-0.48561) | 1 | 1 |
| G: -5312.42844 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.99694 HOMO: -7.15659 LUMO: 0.20681 factor:1 | 1 (-0.20281) | 1 | 1 |
| G: -5312.42844 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.02563 HOMO: -7.11306 LUMO: 0.14150 factor:1 | 1 (-0.23149) | 1 | 1 |
| G: -5312.42844 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.49426 HOMO: -6.67223 LUMO: -0.86260 factor:1 | 1 (-0.70012) | -1 | -1 |
| G: -5312.42844 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.27080 HOMO: -6.92530 LUMO: 0.30749 factor:1 | 1 (-0.47666) | -1 | -1 |
| G: -5312.42844 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.21970 HOMO: -6.50624 LUMO: -0.70477 factor:1 | 1 (-0.42556) | -1 | -1 |
| G: -5312.42844 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.41154 HOMO: -7.35524 LUMO: 0.75103 factor:1 | 1 (-0.61740) | 1 | 1 |
| G: -5312.42844 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.12786 HOMO: -7.07768 LUMO: -0.26939 factor:1 | 1 (-0.33372) | 1 | 1 |
| G: -5312.42844 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.03646 HOMO: -7.15932 LUMO: 0.42450 factor:1 | 1 (-0.24232) | 1 | 1 |
| G: -5312.42844 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.04252 HOMO: -7.46136 LUMO: 0.04626 factor:1 | 1 (-0.24839) | 1 | 1 |
| G: -5312.42844 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.17208 HOMO: -7.05047 LUMO: -1.06669 factor:1 | 1 (-0.37794) | -1 | -1 |
| G: -5312.42844 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.27534 HOMO: -6.66951 LUMO: -0.99322 factor:1 | 1 (-0.48121) | -1 | -1 |
| G: -5312.42844 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.19602 HOMO: -7.01782 LUMO: -1.08846 factor:1 | 1 (-0.40188) | -1 | -1 |
| G: -5312.42844 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.34925 HOMO: -7.03959 LUMO: -1.15376 factor:1 | 1 (-0.55511) | -1 | -1 |
| G: -5312.42844 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.23695 HOMO: -6.68856 LUMO: 1.61364 factor:1 | 1 (-0.44281) | -1 | -1 |
| G: -5312.42844 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.24002 HOMO: -6.53345 LUMO: 1.60275 factor:1 | 1 (-0.44589) | -1 | -1 |
| G: -5312.42844 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.05303 HOMO: -6.73482 LUMO: 1.86398 factor:1 | 1 (-0.25889) | -1 | -1 |
| G: -5312.42844 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.00054 HOMO: -6.87632 LUMO: 1.59731 factor:1 | 1 (-0.20640) | -1 | -1 |
| G: -5312.42844 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.78951 HOMO: -6.31848 LUMO: 2.12521 factor:1 | -1 (0.00463) | -1 | -1 |
| G: -5312.42844 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.03101 HOMO: -6.35114 LUMO: 1.71432 factor:1 | 1 (-0.23688) | -1 | -1 |
| G: -5312.42844 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.20609 HOMO: -6.34842 LUMO: 1.92929 factor:1 | 1 (-0.41195) | -1 | -1 |
| G: -5312.42844 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.03836 HOMO: -6.14977 LUMO: 1.78235 factor:1 | 1 (-0.24422) | -1 | -1 |
| G: -5312.42844 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.91520 HOMO: -6.31032 LUMO: 1.51567 factor:1 | 1 (-0.12106) | -1 | -1 |
| G: -5312.42844 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.18606 HOMO: -6.25862 LUMO: 1.75241 factor:1 | 1 (-0.39193) | -1 | -1 |
| G: -5312.42844 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.73112 HOMO: -6.49264 LUMO: 1.66806 factor:1 | -1 (0.06302) | -1 | -1 |
| G: -5312.42844 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.61925 HOMO: -6.28311 LUMO: 1.60003 factor:1 | -1 (0.17489) | -1 | -1 |
| G: -5312.42844 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.08764 HOMO: -7.13210 LUMO: -0.04354 factor:1 | 1 (-0.29350) | 1 | 1 |
| G: -5312.42844 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.22753 HOMO: -7.35252 LUMO: 0.03537 factor:1 | 1 (-0.43340) | 1 | 1 |
| G: -5312.42844 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.01792 HOMO: -6.58243 LUMO: -0.48980 factor:1 | 1 (-0.22379) | -1 | -1 |
| G: -5312.42844 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.30457 HOMO: -6.90081 LUMO: -0.05442 factor:1 | 1 (-0.51043) | -1 | -1 |
| G: -5312.42844 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.11387 HOMO: -7.22734 LUMO: 0.17143 factor:1 | 1 (-0.31973) | 1 | 1 |
| G: -5312.42844 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.87577 HOMO: -7.13210 LUMO: -0.99866 factor:1 | 1 (-0.08163) | 1 | 1 |
| G: -5312.42844 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.67611 HOMO: -7.39878 LUMO: 0.13334 factor:1 | 1 (-0.88198) | 1 | 1 |
| G: -5312.42844 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.67802 HOMO: -7.04503 LUMO: -0.89798 factor:1 | 1 (-0.88388) | -1 | -1 |
| G: -5312.42844 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.99155 HOMO: -6.95523 LUMO: -1.07213 factor:1 | 1 (-1.19741) | -1 | -1 |
| G: -5312.42844 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.90575 HOMO: -6.75114 LUMO: -1.28438 factor:1 | 1 (-1.11161) | -1 | -1 |
| G: -5312.42844 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.85865 HOMO: -6.75114 LUMO: -0.11701 factor:1 | 1 (-1.06451) | -1 | -1 |
| G: -5312.42844 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.81416 HOMO: -6.83278 LUMO: -0.01633 factor:1 | 1 (-1.02002) | -1 | -1 |
| G: -5312.42844 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11578.01541 HOMO: -6.93890 LUMO: -0.88981 factor:1 | 1 (-1.22127) | -1 | -1 |
| G: -5312.42844 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11578.09452 HOMO: -7.07224 LUMO: -1.08573 factor:1 | 1 (-1.30038) | 1 | 1 |
| G: -5312.42844 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.90474 HOMO: -6.99877 LUMO: -0.95240 factor:1 | 1 (-1.11061) | -1 | -1 |
| G: -5312.42844 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.85944 HOMO: -7.09129 LUMO: 0.35375 factor:1 | 1 (-1.06530) | 1 | 1 |
| G: -5312.42844 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.87750 HOMO: -7.09401 LUMO: 0.04354 factor:1 | 1 (-1.08337) | 1 | 1 |
| G: -5312.42844 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.94532 HOMO: -6.85183 LUMO: -0.68573 factor:1 | 1 (-1.15118) | -1 | -1 |
| G: -5312.42844 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.53225 HOMO: -6.83006 LUMO: -0.58777 factor:1 | 1 (-0.73811) | -1 | -1 |
| G: -5312.42844 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.52909 HOMO: -7.40422 LUMO: 0.17687 factor:1 | 1 (-0.73495) | 1 | 1 |
| G: -5312.42844 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.18925 HOMO: -7.15932 LUMO: 0.10340 factor:1 | 1 (-0.39511) | 1 | 1 |
| G: -5312.42844 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.09014 HOMO: -7.03414 LUMO: -0.19592 factor:1 | 1 (-0.29601) | -1 | -1 |
| G: -5312.42844 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.02601 HOMO: -6.48447 LUMO: -0.36191 factor:1 | 1 (-0.23187) | -1 | -1 |
| G: -5312.42844 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.12761 HOMO: -7.49402 LUMO: 0.11429 factor:1 | 1 (-0.33348) | 1 | 1 |
| G: -5312.42844 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.23515 HOMO: -7.01237 LUMO: -1.06397 factor:1 | 1 (-0.44101) | -1 | -1 |
| G: -5312.42844 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.42912 HOMO: -6.67223 LUMO: -1.07213 factor:1 | 1 (-0.63498) | -1 | -1 |
| G: -5312.42844 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.25564 HOMO: -7.38789 LUMO: -1.15376 factor:1 | 1 (-0.46151) | 1 | 1 |
| G: -5312.42844 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.07262 HOMO: -6.42461 LUMO: -1.23812 factor:1 | 1 (-0.27848) | -1 | -1 |
| G: -5312.42844 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.96851 HOMO: -7.36884 LUMO: -1.19186 factor:1 | 1 (-0.17437) | 1 | 1 |
| G: -5312.42844 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.64830 HOMO: -6.65591 LUMO: 0.07075 factor:1 | 1 (-0.85417) | -1 | -1 |
| G: -5312.42844 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.78792 HOMO: -7.39061 LUMO: -0.16871 factor:1 | 1 (-0.99379) | 1 | 1 |
| G: -5312.42844 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.77935 HOMO: -6.90353 LUMO: -0.96056 factor:1 | 1 (-0.98522) | -1 | -1 |
| G: -5312.42844 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.48000 HOMO: -7.42054 LUMO: 0.19048 factor:1 | 1 (-0.68586) | 1 | 1 |
| G: -5312.42844 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.60520 HOMO: -7.40150 LUMO: 0.35647 factor:1 | 1 (-0.81106) | 1 | 1 |
| G: -5312.42844 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.52966 HOMO: -6.56067 LUMO: -0.96056 factor:1 | 1 (-0.73552) | -1 | -1 |
| G: -5312.42844 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.73465 HOMO: -6.89809 LUMO: -0.81090 factor:1 | 1 (-0.94051) | -1 | -1 |
| G: -5312.42844 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.79674 HOMO: -6.91986 LUMO: -0.84900 factor:1 | 1 (-1.00260) | -1 | -1 |
| G: -5312.42844 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.89661 HOMO: -6.61509 LUMO: -0.62042 factor:1 | 1 (-1.10247) | -1 | -1 |
| G: -5312.42844 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.76188 HOMO: -6.58243 LUMO: -0.65579 factor:1 | 1 (-0.96775) | -1 | -1 |
| G: -5312.42844 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.63121 HOMO: -6.52257 LUMO: -0.92519 factor:1 | 1 (-0.83708) | -1 | -1 |
| G: -5312.42844 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.66942 HOMO: -6.69128 LUMO: 1.49118 factor:1 | 1 (-0.87528) | -1 | -1 |
| G: -5312.42844 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.44680 HOMO: -7.02870 LUMO: 1.67894 factor:1 | 1 (-0.65267) | -1 | -1 |
| G: -5312.42844 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.38041 HOMO: -6.88720 LUMO: 1.68711 factor:1 | 1 (-0.58627) | -1 | -1 |
| G: -5312.42844 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.87582 HOMO: -5.89943 LUMO: 1.03675 factor:1 | 1 (-1.08168) | -1 | -1 |
| G: -5312.42844 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.78741 HOMO: -6.40556 LUMO: 1.14560 factor:1 | 1 (-0.99327) | -1 | -1 |
| G: -5312.42844 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.57883 HOMO: -6.51168 LUMO: 1.48030 factor:1 | 1 (-0.78469) | -1 | -1 |
| G: -5312.42844 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.53548 HOMO: -6.64502 LUMO: 1.91568 factor:1 | 1 (-0.74135) | -1 | -1 |
| G: -5312.42844 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.71884 HOMO: -6.47903 LUMO: 1.91296 factor:1 | 1 (-0.92470) | -1 | -1 |
| G: -5312.42844 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.56027 HOMO: -6.34297 LUMO: 1.91840 factor:1 | 1 (-0.76614) | -1 | -1 |
| G: -5312.42844 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.60539 HOMO: -6.89809 LUMO: 1.82861 factor:1 | 1 (-0.81125) | -1 | -1 |
| G: -5312.42844 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.86542 HOMO: -6.10079 LUMO: 1.62996 factor:1 | 1 (-1.07129) | -1 | -1 |
| G: -5312.42844 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.84153 HOMO: -7.16476 LUMO: -0.92247 factor:1 | 1 (-1.04739) | 1 | 1 |
| G: -5312.42844 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.79122 HOMO: -7.10489 LUMO: -0.95784 factor:1 | 1 (-0.99708) | 1 | 1 |
| G: -5312.42844 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.86757 HOMO: -6.76475 LUMO: -0.99866 factor:1 | 1 (-1.07343) | -1 | -1 |
| G: -5312.42844 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.44610 HOMO: -6.81373 LUMO: -1.05036 factor:1 | 1 (-0.65196) | -1 | -1 |
| G: -5312.42844 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.48253 HOMO: -6.90081 LUMO: -1.03947 factor:1 | 1 (-0.68839) | -1 | -1 |
| G: -5312.42844 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11578.00534 HOMO: -7.06952 LUMO: -0.91702 factor:1 | 1 (-1.21121) | 1 | 1 |
| G: -5312.42844 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.02437 HOMO: -6.73482 LUMO: -0.94151 factor:1 | 1 (-0.23024) | -1 | -1 |
| G: -5312.42844 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.83112 HOMO: -6.99605 LUMO: -1.04764 factor:1 | 1 (-0.03698) | -1 | -1 |
| G: -5312.42844 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.03741 HOMO: -7.03686 LUMO: -0.93335 factor:1 | 1 (-0.24327) | -1 | -1 |
| G: -5312.42844 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.16111 HOMO: -6.81101 LUMO: -0.95240 factor:1 | 1 (-0.36697) | -1 | -1 |
| G: -5312.42844 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.77963 HOMO: -6.83822 LUMO: -0.65307 factor:1 | -1 (0.01450) | -1 | -1 |
| G: -5312.42844 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.97368 HOMO: -7.05319 LUMO: -0.81634 factor:1 | 1 (-0.17954) | -1 | -1 |
| G: -5312.42844 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.91398 HOMO: -7.57565 LUMO: 0.19048 factor:1 | 1 (-0.11984) | 1 | 1 |
| G: -5312.42844 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.86132 HOMO: -6.56067 LUMO: -0.50613 factor:1 | 1 (-0.06718) | -1 | -1 |
| G: -5312.42844 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.74589 HOMO: -6.74298 LUMO: -0.70477 factor:1 | -1 (0.04825) | -1 | -1 |
| G: -5312.42844 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.68246 HOMO: -7.02054 LUMO: 0.03537 factor:1 | -1 (0.11168) | -1 | -1 |
| G: -5312.42844 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.05036 HOMO: -7.33347 LUMO: -0.17960 factor:1 | 1 (-0.25622) | 1 | 1 |
| G: -5312.42844 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.90026 HOMO: -6.98244 LUMO: -0.88165 factor:1 | 1 (-0.10612) | -1 | -1 |
| G: -5312.42844 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.29856 HOMO: -7.14843 LUMO: -1.19730 factor:1 | 1 (-0.50442) | 1 | 1 |
| G: -5312.42844 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.01833 HOMO: -7.17564 LUMO: -1.21907 factor:1 | 1 (-0.22419) | 1 | 1 |
| G: -5312.42844 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.92728 HOMO: -6.74026 LUMO: -0.86532 factor:1 | 1 (-0.13315) | -1 | -1 |
| G: -5312.42844 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.89828 HOMO: -6.82462 LUMO: -1.24084 factor:1 | 1 (-0.10414) | -1 | -1 |
| G: -5312.42844 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.85180 HOMO: -6.78924 LUMO: -0.70477 factor:1 | 1 (-0.05766) | -1 | -1 |
| G: -5312.42844 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.98070 HOMO: -7.41238 LUMO: 0.05987 factor:1 | 1 (-0.18656) | 1 | 1 |
| G: -5312.42844 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.20810 HOMO: -6.75931 LUMO: 0.02721 factor:1 | 1 (-0.41397) | -1 | -1 |
| G: -5312.42844 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.69237 HOMO: -6.28583 LUMO: -0.93063 factor:1 | -1 (0.10177) | -1 | -1 |
| G: -5312.42844 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.96824 HOMO: -6.69128 LUMO: -0.83539 factor:1 | 1 (-0.17410) | -1 | -1 |
| G: -5312.42844 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.09997 HOMO: -7.22190 LUMO: 0.01361 factor:1 | 1 (-0.30583) | 1 | 1 |
| G: -5312.42844 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.91844 HOMO: -6.95251 LUMO: -1.09934 factor:1 | 1 (-0.12430) | -1 | -1 |
| G: -5312.42844 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.90443 HOMO: -6.75387 LUMO: -0.90614 factor:1 | 1 (-0.11029) | -1 | -1 |
| G: -5312.42844 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.82214 HOMO: -7.48585 LUMO: 0.05987 factor:1 | 1 (-0.02800) | 1 | 1 |
| G: -5312.42844 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.06573 HOMO: -6.92802 LUMO: -0.66940 factor:1 | 1 (-0.27160) | -1 | -1 |
| G: -5312.42844 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.81558 HOMO: -7.29537 LUMO: -0.14150 factor:1 | 1 (-0.02144) | 1 | 1 |
| G: -5312.42844 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.76570 HOMO: -6.57155 LUMO: -0.86804 factor:1 | -1 (0.02844) | -1 | -1 |
| G: -5312.42844 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.68400 HOMO: -6.87632 LUMO: -0.77825 factor:1 | 1 (-0.88987) | -1 | -1 |
| G: -5312.42844 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.88300 HOMO: -6.45998 LUMO: -0.31565 factor:1 | 1 (-1.08886) | -1 | -1 |
| G: -5312.42844 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.80422 HOMO: -7.51306 LUMO: 0.05714 factor:1 | 1 (-1.01009) | 1 | 1 |
| G: -5312.42844 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.33064 HOMO: -6.86271 LUMO: -0.00816 factor:1 | 1 (-0.53650) | -1 | -1 |
| G: -5312.42844 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.75894 HOMO: -6.43277 LUMO: -1.07485 factor:1 | 1 (-0.96481) | -1 | -1 |
| G: -5312.42844 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.47532 HOMO: -6.78108 LUMO: -0.81362 factor:1 | 1 (-0.68118) | -1 | -1 |
| G: -5312.42844 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.45513 HOMO: -6.88448 LUMO: 1.21907 factor:1 | 1 (-0.66099) | -1 | -1 |
| G: -5312.42844 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.65290 HOMO: -6.97700 LUMO: 1.44765 factor:1 | 1 (-0.85876) | -1 | -1 |
| G: -5312.42844 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.93150 HOMO: -6.89537 LUMO: 2.12249 factor:1 | 1 (-0.13736) | -1 | -1 |
| G: -5312.42844 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.92059 HOMO: -6.28311 LUMO: 1.45037 factor:1 | 1 (-0.12645) | -1 | -1 |
| G: -5312.42844 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.20541 HOMO: -6.55522 LUMO: 1.39867 factor:1 | 1 (-0.41127) | -1 | -1 |
| G: -5312.42844 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.73593 HOMO: -6.46815 LUMO: 1.50207 factor:1 | -1 (0.05821) | -1 | -1 |
| G: -5312.42844 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.74094 HOMO: -6.43549 LUMO: 2.17419 factor:1 | -1 (0.05320) | -1 | -1 |
| G: -5312.42844 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.04489 HOMO: -6.99333 LUMO: 1.87214 factor:1 | 1 (-0.25075) | -1 | -1 |
| G: -5312.42844 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.92568 HOMO: -6.65591 LUMO: 1.37962 factor:1 | 1 (-0.13154) | -1 | -1 |
| G: -5312.42844 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.98187 HOMO: -6.82734 LUMO: 1.55649 factor:1 | 1 (-0.18773) | -1 | -1 |
| G: -5312.42844 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.27722 HOMO: -6.71849 LUMO: 1.36057 factor:1 | 1 (-0.48308) | -1 | -1 |
| G: -5312.42844 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.82358 HOMO: -6.79468 LUMO: 1.82044 factor:1 | 1 (-0.02944) | -1 | -1 |
| G: -5312.42844 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.57054 HOMO: -6.61237 LUMO: 1.15104 factor:1 | -1 (0.22360) | -1 | -1 |
| G: -5312.42844 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.08184 HOMO: -6.62053 LUMO: 2.33474 factor:1 | 1 (-0.28771) | -1 | -1 |
| G: -5312.42844 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.70129 HOMO: -6.55794 LUMO: 1.65717 factor:1 | -1 (0.09285) | -1 | -1 |
| G: -5312.42844 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.94511 HOMO: -6.85999 LUMO: 2.03813 factor:1 | 1 (-0.15097) | -1 | -1 |
| G: -5312.42844 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.06628 HOMO: -6.45726 LUMO: 1.28438 factor:1 | 1 (-0.27214) | -1 | -1 |
| G: -5312.42844 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.78309 HOMO: -6.23685 LUMO: 1.93201 factor:1 | -1 (0.01105) | -1 | -1 |
| G: -5312.42844 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.83762 HOMO: -7.06680 LUMO: 1.86942 factor:1 | 1 (-0.04348) | 1 | 1 |
| G: -5312.42844 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.66676 HOMO: -6.89537 LUMO: 2.17147 factor:1 | -1 (0.12738) | -1 | -1 |
| G: -5312.42844 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.03112 HOMO: -6.80013 LUMO: 1.78779 factor:1 | 1 (-0.23698) | -1 | -1 |
| G: -5312.42844 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.22819 HOMO: -6.45726 LUMO: 1.58370 factor:1 | 1 (-0.43405) | -1 | -1 |
| G: -5312.42844 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.85466 HOMO: -6.52529 LUMO: 1.71976 factor:1 | 1 (-0.06052) | -1 | -1 |
| G: -5312.42844 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.01031 HOMO: -7.22462 LUMO: -1.18642 factor:1 | 1 (-0.21617) | 1 | 1 |
| G: -5312.42844 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.97088 HOMO: -7.18381 LUMO: -0.78641 factor:1 | 1 (-0.17674) | 1 | 1 |
| G: -5312.42844 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.19308 HOMO: -6.93346 LUMO: 1.65717 factor:1 | 1 (-0.39895) | -1 | -1 |
| G: -5312.42844 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.08269 HOMO: -6.41644 LUMO: 1.78235 factor:1 | 1 (-0.28855) | -1 | -1 |
| G: -5312.42844 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.92135 HOMO: -6.59876 LUMO: 1.83677 factor:1 | 1 (-0.12721) | -1 | -1 |
| G: -5312.42844 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.92456 HOMO: -6.35658 LUMO: 1.59731 factor:1 | 1 (-0.13042) | -1 | -1 |
| G: -5312.42844 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.84701 HOMO: -6.60692 LUMO: 1.66534 factor:1 | 1 (-0.05287) | -1 | -1 |
| G: -5312.42844 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.89330 HOMO: -6.83006 LUMO: 2.11705 factor:1 | 1 (-0.09916) | -1 | -1 |
| G: -5312.42844 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.72197 HOMO: -6.89264 LUMO: 1.30070 factor:1 | -1 (0.07216) | -1 | -1 |
| G: -5312.42844 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.94451 HOMO: -6.90081 LUMO: 2.05174 factor:1 | 1 (-0.15037) | -1 | -1 |
| G: -5312.42844 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.79626 HOMO: -6.74842 LUMO: 1.96194 factor:1 | 1 (-0.00212) | -1 | -1 |
| G: -5312.42844 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.07939 HOMO: -6.58516 LUMO: 1.30887 factor:1 | 1 (-0.28526) | -1 | -1 |
| G: -5312.42844 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.96478 HOMO: -7.00965 LUMO: 2.08167 factor:1 | 1 (-0.17064) | -1 | -1 |
| G: -5312.42844 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.76636 HOMO: -6.86815 LUMO: 2.29664 factor:1 | -1 (0.02778) | -1 | -1 |
| G: -5312.42844 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.13714 HOMO: -6.39740 LUMO: 2.02725 factor:1 | 1 (-0.34300) | -1 | -1 |
| G: -5312.42844 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.75381 HOMO: -5.95929 LUMO: 1.62724 factor:1 | -1 (0.04033) | -1 | -1 |
| G: -5312.42844 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.68619 HOMO: -6.71849 LUMO: 1.34696 factor:1 | -1 (0.10795) | -1 | -1 |
| G: -5312.42844 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.49944 HOMO: -7.26816 LUMO: 1.74153 factor:1 | -1 (0.29470) | 1 | 1 |
| G: -5312.42844 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.92116 HOMO: -6.90897 LUMO: 1.71432 factor:1 | 1 (-0.12702) | -1 | -1 |
| G: -5312.42844 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.03504 HOMO: -6.70489 LUMO: 1.91568 factor:1 | 1 (-0.24090) | -1 | -1 |
| G: -5312.42844 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.07667 HOMO: -6.83278 LUMO: 1.61908 factor:1 | 1 (-0.28254) | -1 | -1 |
| G: -5312.42844 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.74293 HOMO: -7.17292 LUMO: 1.95378 factor:1 | -1 (0.05121) | 1 | -1 |
| G: -5312.42844 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.64899 HOMO: -6.53345 LUMO: 1.74153 factor:1 | -1 (0.14515) | -1 | -1 |
| G: -5312.42844 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.11213 HOMO: -6.53073 LUMO: 1.51023 factor:1 | 1 (-0.31799) | -1 | -1 |
| G: -5312.42844 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.13232 HOMO: -6.93346 LUMO: 2.22861 factor:1 | 1 (-0.33818) | -1 | -1 |
| G: -5312.42844 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.21714 HOMO: -6.47903 LUMO: 2.05446 factor:1 | 1 (-0.42300) | -1 | -1 |
| G: -5312.42844 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.27488 HOMO: -6.88992 LUMO: 1.57010 factor:1 | 1 (-0.48074) | -1 | -1 |
| G: -5312.42844 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.01229 HOMO: -6.07358 LUMO: 1.95922 factor:1 | 1 (-0.21815) | -1 | -1 |
| G: -5312.42844 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.12990 HOMO: -6.75114 LUMO: 2.18780 factor:1 | 1 (-0.33576) | -1 | -1 |
| G: -5312.42844 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.98062 HOMO: -6.96339 LUMO: 1.70071 factor:1 | 1 (-0.18648) | -1 | -1 |
| G: -5312.42844 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.63745 HOMO: -7.14843 LUMO: 1.82588 factor:1 | 1 (-0.84331) | 1 | -1 |
| G: -5312.42844 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.52874 HOMO: -6.96339 LUMO: 2.29392 factor:1 | 1 (-0.73460) | -1 | -1 |
| G: -5312.42844 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.70515 HOMO: -6.81645 LUMO: 2.39732 factor:1 | 1 (-0.91101) | -1 | -1 |
| G: -5312.42844 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.89748 HOMO: -6.48447 LUMO: 1.24084 factor:1 | 1 (-1.10334) | -1 | -1 |
| G: -5312.42844 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.57842 HOMO: -7.14843 LUMO: 2.01092 factor:1 | 1 (-0.78429) | 1 | -1 |
| G: -5312.42844 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.45472 HOMO: -7.20013 LUMO: -0.34286 factor:1 | 1 (-0.66058) | 1 | -1 |
| G: -5312.42844 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.96644 HOMO: -6.97700 LUMO: -0.15238 factor:1 | 1 (-0.17230) | -1 | -1 |
| G: -5312.42844 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.98712 HOMO: -7.07768 LUMO: -0.26123 factor:1 | 1 (-0.19298) | 1 | -1 |
| G: -5312.42844 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.79120 HOMO: -6.99333 LUMO: -0.41361 factor:1 | -1 (0.00294) | -1 | -1 |
| G: -5312.42844 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.68412 HOMO: -6.84638 LUMO: -0.40273 factor:1 | -1 (0.11002) | -1 | -1 |
| G: -5312.42844 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.41359 HOMO: -6.83822 LUMO: -0.26939 factor:1 | -1 (0.38055) | -1 | -1 |
| G: -5312.42844 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.86970 HOMO: -6.75931 LUMO: -0.93879 factor:1 | 1 (-0.07557) | -1 | -1 |
| G: -5312.42844 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.60431 HOMO: -6.79468 LUMO: -0.39729 factor:1 | -1 (0.18983) | -1 | -1 |
| G: -5312.42844 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.29957 HOMO: -6.93890 LUMO: 0.43266 factor:1 | -1 (0.49457) | -1 | -1 |
| G: -5312.42844 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.16326 HOMO: -7.08040 LUMO: -0.85716 factor:1 | 1 (-0.36912) | 1 | 1 |
| G: -5312.42844 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.08745 HOMO: -6.70216 LUMO: -1.41499 factor:1 | 1 (-0.29331) | -1 | -1 |
| G: -5312.42844 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.26451 HOMO: -6.63686 LUMO: -0.52790 factor:1 | 1 (-0.47038) | -1 | -1 |
| G: -5312.42844 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.38332 HOMO: -6.75114 LUMO: -0.13334 factor:1 | 1 (-0.58918) | -1 | -1 |
| G: -5312.42844 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.39948 HOMO: -6.94435 LUMO: -0.24490 factor:1 | 1 (-0.60534) | -1 | -1 |
| G: -5312.42844 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.03632 HOMO: -6.74298 LUMO: -0.84627 factor:1 | 1 (-0.24218) | -1 | -1 |
| G: -5312.42844 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.09812 HOMO: -7.15932 LUMO: 0.22041 factor:1 | 1 (-0.30398) | 1 | 1 |
| G: -5312.42844 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.94685 HOMO: -6.90081 LUMO: -1.16737 factor:1 | 1 (-0.15271) | -1 | -1 |
| G: -5312.42844 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.28601 HOMO: -7.04775 LUMO: -0.84355 factor:1 | 1 (-0.49187) | -1 | -1 |
| G: -5312.42844 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.99713 HOMO: -7.17020 LUMO: -1.31159 factor:1 | 1 (-0.20300) | 1 | 1 |
| G: -5312.42844 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.09074 HOMO: -7.14571 LUMO: -0.46259 factor:1 | 1 (-0.29660) | 1 | 1 |
| G: -5312.42844 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.34656 HOMO: -7.45048 LUMO: -0.91158 factor:1 | 1 (-0.55242) | 1 | 1 |
| G: -5312.42844 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.19115 HOMO: -6.87360 LUMO: -0.82995 factor:1 | 1 (-0.39701) | -1 | -1 |
| G: -5312.42844 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.84086 HOMO: -7.43415 LUMO: -0.65307 factor:1 | 1 (-0.04672) | 1 | 1 |
| G: -5312.42844 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.68709 HOMO: -7.47225 LUMO: -0.77280 factor:1 | -1 (0.10705) | 1 | 1 |
| G: -5312.42844 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.80132 HOMO: -6.86271 LUMO: -0.83811 factor:1 | 1 (-0.00718) | -1 | -1 |
| G: -5312.42844 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.69625 HOMO: -7.53483 LUMO: -0.66124 factor:1 | 1 (-0.90211) | 1 | 1 |
| G: -5312.42844 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.81827 HOMO: -7.45864 LUMO: -1.08301 factor:1 | 1 (-1.02413) | 1 | 1 |
| G: -5312.42844 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.88526 HOMO: -7.24639 LUMO: -1.19186 factor:1 | 1 (-1.09112) | 1 | 1 |
| G: -5312.42844 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.88980 HOMO: -7.54844 LUMO: -0.96873 factor:1 | 1 (-1.09567) | 1 | 1 |
| G: -5312.42844 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11578.06652 HOMO: -7.12666 LUMO: -0.01633 factor:1 | 1 (-1.27238) | 1 | 1 |
| G: -5312.42844 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.83829 HOMO: -6.77291 LUMO: -0.70477 factor:1 | 1 (-1.04416) | -1 | -1 |
| G: -5312.42844 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.65535 HOMO: -6.76475 LUMO: -1.15921 factor:1 | 1 (-0.86121) | -1 | -1 |
| G: -5312.42844 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.04835 HOMO: -5.37697 LUMO: -0.56600 factor:1 | 1 (-0.25421) | -1 | -1 |
| G: -5312.42844 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.15640 HOMO: -6.62053 LUMO: -1.75513 factor:1 | 1 (-0.36227) | -1 | -1 |
| G: -5312.42844 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.17488 HOMO: -6.60420 LUMO: -1.74697 factor:1 | 1 (-0.38074) | -1 | -1 |
| G: -5312.42844 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.31189 HOMO: -6.84366 LUMO: -0.94968 factor:1 | 1 (-0.51775) | -1 | -1 |
| G: -5312.42844 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.35012 HOMO: -6.96884 LUMO: -2.11977 factor:1 | 1 (-0.55598) | -1 | -1 |
| G: -5312.42844 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.09091 HOMO: -6.80829 LUMO: 0.56055 factor:1 | 1 (-0.29677) | -1 | -1 |
| G: -5312.42844 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.99406 HOMO: -7.02326 LUMO: 0.11429 factor:1 | 1 (-0.19992) | -1 | -1 |
| G: -5312.42844 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.75104 HOMO: -7.40966 LUMO: 0.18232 factor:1 | -1 (0.04310) | 1 | 1 |
| G: -5312.42844 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.06114 HOMO: -6.34570 LUMO: 0.41089 factor:1 | 1 (-0.26700) | -1 | -1 |
| G: -5312.42844 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.94192 HOMO: -6.78924 LUMO: 0.49525 factor:1 | 1 (-0.14779) | -1 | -1 |
| G: -5312.42844 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.88837 HOMO: -6.87632 LUMO: 0.44082 factor:1 | 1 (-0.09423) | -1 | -1 |
| G: -5312.42844 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.07659 HOMO: -6.69944 LUMO: 1.20546 factor:1 | 1 (-0.28245) | -1 | -1 |
| G: -5312.42844 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.91991 HOMO: -6.83006 LUMO: 1.28982 factor:1 | 1 (-0.12577) | -1 | -1 |
| G: -5312.42844 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.06304 HOMO: -7.78246 LUMO: 0.20681 factor:1 | 1 (-0.26890) | 1 | 1 |
| G: -5312.42844 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.96138 HOMO: -6.55794 LUMO: -1.65173 factor:1 | 1 (-0.16724) | -1 | -1 |
| G: -5312.42844 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.70750 HOMO: -6.77564 LUMO: -1.14560 factor:1 | -1 (0.08664) | -1 | -1 |
| G: -5312.42844 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.84739 HOMO: -7.46680 LUMO: -1.18097 factor:1 | 1 (-0.05325) | 1 | 1 |
| G: -5312.42844 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.58676 HOMO: -6.88176 LUMO: -1.24900 factor:1 | -1 (0.20738) | -1 | -1 |
| G: -5312.42844 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.81666 HOMO: -7.28177 LUMO: -0.42178 factor:1 | 1 (-1.02252) | 1 | 1 |
| G: -5312.42844 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.73437 HOMO: -7.71715 LUMO: 0.19592 factor:1 | 1 (-0.94024) | 1 | 1 |
| G: -5312.42844 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.79914 HOMO: -7.02326 LUMO: -1.40683 factor:1 | 1 (-1.00500) | -1 | -1 |
| G: -5312.42844 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.63399 HOMO: -7.27088 LUMO: -1.07485 factor:1 | 1 (-0.83985) | 1 | 1 |
| G: -5312.42844 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.89179 HOMO: -7.17020 LUMO: -0.49525 factor:1 | 1 (-1.09765) | 1 | 1 |
| G: -5312.42844 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.87125 HOMO: -7.15932 LUMO: 0.02721 factor:1 | 1 (-1.07711) | 1 | 1 |
| G: -5312.42844 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11578.06064 HOMO: -7.00693 LUMO: -0.83267 factor:1 | 1 (-1.26650) | -1 | -1 |
| G: -5312.42844 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.61208 HOMO: -6.86543 LUMO: -0.10340 factor:1 | 1 (-0.81795) | -1 | -1 |
| G: -5312.42844 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.62373 HOMO: -7.11850 LUMO: -0.08980 factor:1 | 1 (-0.82959) | 1 | 1 |
| G: -5312.42844 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.53227 HOMO: -6.87087 LUMO: -0.88981 factor:1 | 1 (-0.73814) | -1 | -1 |
| G: -5312.42844 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.94232 HOMO: -7.08857 LUMO: -1.27077 factor:1 | 1 (-1.14818) | 1 | 1 |
| G: -5312.42844 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.12125 HOMO: -6.79468 LUMO: -0.81906 factor:1 | 1 (-0.32711) | -1 | -1 |
| G: -5312.42844 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.03354 HOMO: -6.86815 LUMO: -0.89798 factor:1 | 1 (-0.23941) | -1 | -1 |
| G: -5312.42844 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.34838 HOMO: -6.78652 LUMO: -2.00548 factor:1 | 1 (-0.55424) | -1 | -1 |
| G: -5312.42844 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.90081 HOMO: -6.75114 LUMO: -0.08436 factor:1 | 1 (-0.10667) | -1 | -1 |
| G: -5312.42844 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.73860 HOMO: -6.55794 LUMO: 0.52790 factor:1 | -1 (0.05554) | -1 | -1 |
| G: -5312.42844 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.93972 HOMO: -7.17836 LUMO: 0.28300 factor:1 | 1 (-0.14558) | 1 | -1 |
| G: -5312.42844 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.95477 HOMO: -7.35796 LUMO: -0.77552 factor:1 | 1 (-0.16063) | 1 | 1 |
| G: -5312.42844 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.23238 HOMO: -7.23551 LUMO: -1.17553 factor:1 | 1 (-0.43824) | 1 | 1 |
| G: -5312.42844 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.09940 HOMO: -7.07496 LUMO: -1.14288 factor:1 | 1 (-0.30526) | 1 | 1 |
| G: -5312.42844 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.70935 HOMO: -6.70489 LUMO: -0.83539 factor:1 | -1 (0.08479) | -1 | -1 |
| G: -5312.42844 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.63765 HOMO: -6.59604 LUMO: -0.89798 factor:1 | -1 (0.15649) | -1 | -1 |
| G: -5312.42844 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.10530 HOMO: -6.94162 LUMO: -1.22451 factor:1 | 1 (-0.31116) | -1 | -1 |
| G: -5312.42844 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.99441 HOMO: -6.68040 LUMO: 0.22041 factor:1 | 1 (-0.20028) | -1 | -1 |
| G: -5312.42844 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.93267 HOMO: -6.88176 LUMO: 0.11157 factor:1 | 1 (-0.13853) | -1 | -1 |
| G: -5312.42844 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.20152 HOMO: -6.91713 LUMO: 1.27621 factor:1 | 1 (-0.40738) | -1 | -1 |
| G: -5312.42844 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.25621 HOMO: -6.77836 LUMO: 1.01226 factor:1 | 1 (-0.46208) | -1 | -1 |
| G: -5312.42844 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.79329 HOMO: -7.14571 LUMO: 1.48574 factor:1 | -1 (0.00084) | 1 | 1 |
| G: -5312.42844 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.80742 HOMO: -6.96884 LUMO: 1.48574 factor:1 | 1 (-0.01328) | -1 | -1 |
| G: -5312.42844 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.01920 HOMO: -7.24367 LUMO: 1.28438 factor:1 | 1 (-0.22507) | 1 | 1 |
| G: -5312.42844 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.68891 HOMO: -7.10489 LUMO: 1.29526 factor:1 | -1 (0.10523) | 1 | 1 |
| G: -5312.42844 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.49084 HOMO: -7.07224 LUMO: 1.29254 factor:1 | -1 (0.30330) | 1 | 1 |
| G: -5312.42844 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.67669 HOMO: -7.12938 LUMO: 0.49253 factor:1 | -1 (0.11744) | 1 | 1 |
| G: -5312.42844 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.59922 HOMO: -7.33619 LUMO: 1.45581 factor:1 | -1 (0.19492) | 1 | 1 |
| G: -5312.42844 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.93433 HOMO: -6.87904 LUMO: -0.14422 factor:1 | 1 (-0.14019) | -1 | -1 |
| G: -5312.42844 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.64290 HOMO: -6.81917 LUMO: 0.50341 factor:1 | -1 (0.15124) | -1 | -1 |
| G: -5312.42844 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.13787 HOMO: -7.27905 LUMO: 0.13606 factor:1 | 1 (-0.34373) | 1 | -1 |
| G: -5312.42844 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.85610 HOMO: -6.87904 LUMO: -0.09796 factor:1 | 1 (-0.06196) | -1 | -1 |
| G: -5312.42844 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.02211 HOMO: -7.33891 LUMO: 0.03810 factor:1 | 1 (-0.22798) | 1 | 1 |
| G: -5312.42844 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.09765 HOMO: -6.98516 LUMO: 0.98233 factor:1 | 1 (-0.30352) | -1 | -1 |
| G: -5312.42844 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.72420 HOMO: -6.94162 LUMO: 0.86804 factor:1 | -1 (0.06993) | -1 | -1 |
| G: -5312.42844 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.97920 HOMO: -7.37701 LUMO: 0.05442 factor:1 | 1 (-0.18506) | 1 | 1 |
| G: -5312.42844 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.78480 HOMO: -7.04775 LUMO: 0.43266 factor:1 | -1 (0.00933) | -1 | -1 |
| G: -5312.42844 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.86992 HOMO: -7.47497 LUMO: 0.31837 factor:1 | 1 (-0.07578) | 1 | 1 |
| G: -5312.42844 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.14786 HOMO: -6.62053 LUMO: 0.13061 factor:1 | 1 (-0.35372) | -1 | -1 |
| G: -5312.42844 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.73572 HOMO: -6.44366 LUMO: -0.04354 factor:1 | -1 (0.05842) | -1 | -1 |
| G: -5312.42844 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.45800 HOMO: -6.40284 LUMO: 0.68301 factor:1 | -1 (0.33614) | -1 | -1 |
| G: -5312.42844 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.77854 HOMO: -6.73754 LUMO: 0.36735 factor:1 | 1 (-0.98440) | -1 | -1 |
| G: -5312.42844 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.95933 HOMO: -6.85455 LUMO: 0.23946 factor:1 | 1 (-1.16519) | -1 | -1 |
| G: -5312.42844 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.75620 HOMO: -6.93346 LUMO: 0.24762 factor:1 | 1 (-0.96206) | -1 | -1 |
| G: -5312.42844 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.81748 HOMO: -6.85455 LUMO: 0.17687 factor:1 | 1 (-1.02334) | -1 | -1 |
| G: -5312.42844 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.87786 HOMO: -6.62325 LUMO: 0.69933 factor:1 | 1 (-1.08372) | -1 | -1 |
| G: -5312.42844 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11578.09582 HOMO: -6.43005 LUMO: 0.50069 factor:1 | 1 (-1.30168) | -1 | -1 |
| G: -5312.42844 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11578.06219 HOMO: -6.56883 LUMO: 0.22858 factor:1 | 1 (-1.26805) | -1 | -1 |
| G: -5312.42844 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.79258 HOMO: -6.78380 LUMO: 0.54967 factor:1 | 1 (-0.99844) | -1 | -1 |
| G: -5312.42844 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.97930 HOMO: -7.35524 LUMO: 0.00272 factor:1 | 1 (-1.18516) | 1 | 1 |
| G: -5312.42844 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.65464 HOMO: -7.27360 LUMO: 0.08436 factor:1 | 1 (-0.86051) | 1 | 1 |
| G: -5312.42844 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.59236 HOMO: -7.44504 LUMO: -0.96056 factor:1 | 1 (-0.79822) | 1 | 1 |
| G: -5312.42844 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.58583 HOMO: -7.27360 LUMO: 0.29933 factor:1 | 1 (-0.79169) | 1 | 1 |
| G: -5312.42844 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.70866 HOMO: -7.09129 LUMO: 0.41089 factor:1 | 1 (-0.91452) | 1 | 1 |
| G: -5312.42844 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.61007 HOMO: -6.93618 LUMO: 0.36463 factor:1 | 1 (-0.81593) | -1 | -1 |
| G: -5312.42844 HOMO: -7.26000 LUMO: -3.02863 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.45736 HOMO: -7.65728 LUMO: 0.20136 factor:1 | 1 (-0.66322) | 1 | 1 |
| G: -5312.42844 HOMO: -7.26000 LUMO: -3.02863 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.84159 HOMO: -6.90353 LUMO: -0.92791 factor:1 | 1 (-1.04745) | -1 | -1 |
| G: -5312.42844 HOMO: -7.26000 LUMO: -3.02863 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.73775 HOMO: -6.82462 LUMO: -1.18370 factor:1 | 1 (-0.94361) | -1 | -1 |
| G: -5312.42844 HOMO: -7.26000 LUMO: -3.02863 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.76866 HOMO: -7.09129 LUMO: -0.13334 factor:1 | 1 (-0.97452) | 1 | 1 |
| G: -5312.42844 HOMO: -7.26000 LUMO: -3.02863 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.69198 HOMO: -7.40966 LUMO: -1.06941 factor:1 | 1 (-0.89784) | 1 | 1 |
| G: -5312.42844 HOMO: -7.26000 LUMO: -3.02863 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.64398 HOMO: -7.24367 LUMO: -1.00954 factor:1 | 1 (-0.84984) | 1 | 1 |
| G: -5312.42844 HOMO: -7.26000 LUMO: -3.02863 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.45382 HOMO: -7.51851 LUMO: 0.09796 factor:1 | 1 (-0.65969) | 1 | 1 |
| G: -5312.42844 HOMO: -7.26000 LUMO: -3.02863 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.45067 HOMO: -7.48857 LUMO: -0.07619 factor:1 | 1 (-0.65653) | 1 | 1 |
| G: -5312.42844 HOMO: -7.26000 LUMO: -3.02863 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.73813 HOMO: -6.53345 LUMO: 1.09390 factor:1 | 1 (-0.94399) | -1 | -1 |
| G: -5312.42844 HOMO: -7.26000 LUMO: -3.02863 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.61706 HOMO: -7.21918 LUMO: 0.08436 factor:1 | 1 (-0.82293) | 1 | 1 |
| G: -5312.42844 HOMO: -7.26000 LUMO: -3.02863 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.77612 HOMO: -7.38789 LUMO: 1.02587 factor:1 | 1 (-0.98198) | 1 | -1 |
| G: -5312.42844 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.90036 HOMO: -6.83550 LUMO: -0.67484 factor:1 | 1 (-1.10622) | -1 | -1 |
| G: -5312.42844 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.63804 HOMO: -7.04231 LUMO: 0.54151 factor:1 | 1 (-0.84391) | -1 | -1 |
| G: -5312.42844 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: 1.91296 factor:1 | 1 (-0.90002) | 1 | 1 |
| G: -5312.42844 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.90746 HOMO: -7.35796 LUMO: -1.04220 factor:1 | 1 (-1.11333) | -1 | -1 |
| G: -5312.42844 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.72390 HOMO: -6.62597 LUMO: -0.44082 factor:1 | 1 (-0.92976) | -1 | -1 |
| G: -5312.42844 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.56887 HOMO: -6.45182 LUMO: -0.20409 factor:1 | 1 (-0.77474) | -1 | -1 |
| G: -5312.42844 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.67791 HOMO: -6.51168 LUMO: -0.23130 factor:1 | 1 (-0.88377) | -1 | -1 |
| G: -5312.42844 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.82305 HOMO: -7.14027 LUMO: 0.49797 factor:1 | 1 (-1.02892) | -1 | -1 |
| G: -5312.42844 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.67788 HOMO: -7.55660 LUMO: 0.24762 factor:1 | 1 (-0.88374) | -1 | -1 |
| G: -5312.42844 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.51148 HOMO: -6.88992 LUMO: -0.64763 factor:1 | 1 (-0.71735) | -1 | -1 |
| G: -5312.42844 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.85220 HOMO: -6.72665 LUMO: -0.45987 factor:1 | 1 (-1.05806) | -1 | -1 |
| G: -5312.42844 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.90191 HOMO: -6.72121 LUMO: -0.58232 factor:1 | 1 (-1.10778) | -1 | -1 |
| G: -5312.42844 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.75690 HOMO: -7.26816 LUMO: 0.32926 factor:1 | 1 (-0.96277) | -1 | -1 |
| G: -5312.42844 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.96763 HOMO: -6.57155 LUMO: -0.53606 factor:1 | 1 (-1.17349) | -1 | -1 |
| G: -5312.42844 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.71554 HOMO: -6.50896 LUMO: -0.43810 factor:1 | 1 (-0.92140) | -1 | -1 |
| G: -5312.42844 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.29466 HOMO: -6.73210 LUMO: -0.51430 factor:1 | 1 (-0.50053) | -1 | -1 |
| G: -5312.42844 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.44297 HOMO: -6.77019 LUMO: -0.62858 factor:1 | 1 (-0.64883) | -1 | -1 |
| G: -5312.42844 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.58400 HOMO: -6.82462 LUMO: -0.67484 factor:1 | 1 (-0.78986) | -1 | -1 |
| G: -5312.42844 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.84418 HOMO: -6.79740 LUMO: -0.55511 factor:1 | 1 (-0.05004) | -1 | -1 |
| G: -5312.42844 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.94143 HOMO: -6.79740 LUMO: -0.67756 factor:1 | 1 (-0.14730) | -1 | -1 |
| G: -5312.42844 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.01006 HOMO: -6.75114 LUMO: -0.55239 factor:1 | 1 (-0.21592) | -1 | -1 |
| G: -5312.42844 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.90769 HOMO: -6.49536 LUMO: -0.25307 factor:1 | 1 (-0.11355) | -1 | -1 |
| G: -5312.42844 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.05496 HOMO: -6.48992 LUMO: -0.25034 factor:1 | 1 (-0.26082) | -1 | -1 |
| G: -5312.42844 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.99221 HOMO: -6.52801 LUMO: -0.28028 factor:1 | 1 (-0.19807) | -1 | -1 |
| G: -5312.42844 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.17472 HOMO: -7.22462 LUMO: 0.52518 factor:1 | 1 (-0.38058) | -1 | -1 |
| G: -5312.42844 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.13744 HOMO: -6.59332 LUMO: -0.27211 factor:1 | 1 (-0.34330) | -1 | -1 |
| G: -5312.42844 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.99251 HOMO: -6.57427 LUMO: -0.16871 factor:1 | 1 (-0.19837) | -1 | -1 |
| G: -5312.42844 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.84116 HOMO: -6.71033 LUMO: 1.59187 factor:1 | 1 (-0.04702) | 1 | 1 |
| G: -5312.42844 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.16936 HOMO: -6.72121 LUMO: 2.00004 factor:1 | 1 (-0.37522) | 1 | 1 |
| G: -5312.42844 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.78358 HOMO: -6.61509 LUMO: 1.55921 factor:1 | -1 (0.01056) | -1 | -1 |
| G: -5312.42844 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.80780 HOMO: -6.55250 LUMO: 1.73064 factor:1 | 1 (-0.01366) | -1 | -1 |
| G: -5312.42844 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.70978 HOMO: -6.66135 LUMO: 2.02181 factor:1 | -1 (0.08436) | 1 | 1 |
| G: -5312.42844 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.79713 HOMO: -6.84911 LUMO: 1.98099 factor:1 | 1 (-0.00299) | 1 | 1 |
| G: -5312.42844 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.78929 HOMO: -6.66679 LUMO: 1.98371 factor:1 | -1 (0.00484) | 1 | 1 |
| G: -5312.42844 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.94217 HOMO: -6.67495 LUMO: 2.04085 factor:1 | 1 (-0.14803) | 1 | 1 |
| G: -5312.42844 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.12008 HOMO: -6.89809 LUMO: 1.95106 factor:1 | 1 (-0.32594) | 1 | 1 |
| G: -5312.42844 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.01882 HOMO: -6.50352 LUMO: 1.88847 factor:1 | 1 (-0.22468) | -1 | -1 |
| G: -5312.42844 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.95409 HOMO: -6.93618 LUMO: 2.00004 factor:1 | 1 (-0.15995) | 1 | 1 |
| G: -5312.42844 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.79112 HOMO: -6.50896 LUMO: 1.73609 factor:1 | -1 (0.00302) | -1 | -1 |
| G: -5312.42844 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.77260 HOMO: -6.69672 LUMO: 2.37283 factor:1 | 1 (-0.97847) | 1 | 1 |
| G: -5312.42844 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.95446 HOMO: -6.65591 LUMO: 2.20684 factor:1 | 1 (-1.16032) | 1 | 1 |
| G: -5312.42844 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.84308 HOMO: -6.23957 LUMO: 1.78507 factor:1 | 1 (-1.04894) | -1 | -1 |
| G: -5312.42844 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.64814 HOMO: -6.35114 LUMO: 1.92112 factor:1 | 1 (-0.85400) | -1 | -1 |
| G: -5312.42844 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.96434 HOMO: -6.53617 LUMO: 1.75241 factor:1 | 1 (-1.17020) | -1 | -1 |
| G: -5312.42844 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.87887 HOMO: -6.60420 LUMO: 1.78779 factor:1 | 1 (-1.08473) | 1 | 1 |
| G: -5312.42844 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11578.05479 HOMO: -7.40422 LUMO: -0.97145 factor:1 | 1 (-1.26065) | -1 | -1 |
| G: -5312.42844 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.74382 HOMO: -6.80013 LUMO: -0.69117 factor:1 | 1 (-0.94968) | -1 | -1 |
| G: -5312.42844 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.70240 HOMO: -6.68040 LUMO: -0.47076 factor:1 | 1 (-0.90826) | -1 | -1 |
| G: -5312.42844 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11578.05517 HOMO: -7.20285 LUMO: -0.66124 factor:1 | 1 (-1.26103) | -1 | -1 |
| G: -5312.42844 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.78167 HOMO: -6.82734 LUMO: -0.60137 factor:1 | 1 (-0.98753) | -1 | -1 |
| G: -5312.42844 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.89421 HOMO: -7.18653 LUMO: 0.59321 factor:1 | 1 (-1.10007) | -1 | -1 |
| G: -5312.42844 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.70341 HOMO: -7.29265 LUMO: 0.48164 factor:1 | 1 (-0.90927) | -1 | -1 |
| G: -5312.42844 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.61546 HOMO: -6.63414 LUMO: -0.25034 factor:1 | 1 (-0.82132) | -1 | -1 |
| G: -5312.42844 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.47061 HOMO: -7.20285 LUMO: 0.53879 factor:1 | 1 (-0.67648) | -1 | -1 |
| G: -5312.42844 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.86670 HOMO: -6.46815 LUMO: -0.21769 factor:1 | 1 (-1.07256) | -1 | -1 |
| G: -5312.42844 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.66833 HOMO: -6.57971 LUMO: -0.18776 factor:1 | 1 (-0.87419) | -1 | -1 |
| G: -5312.42844 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.47921 HOMO: -6.90897 LUMO: 1.91296 factor:1 | 1 (-0.68507) | 1 | 1 |
| G: -5312.42844 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.68082 HOMO: -6.67495 LUMO: 2.04358 factor:1 | 1 (-0.88668) | 1 | 1 |
| G: -5312.42844 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.72773 HOMO: -6.94162 LUMO: 1.73881 factor:1 | 1 (-0.93360) | 1 | 1 |
| G: -5312.42844 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.64346 HOMO: -6.73482 LUMO: 1.95922 factor:1 | 1 (-0.84932) | 1 | 1 |
| G: -5312.42844 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.81846 HOMO: -6.70489 LUMO: 2.04358 factor:1 | 1 (-1.02432) | 1 | 1 |
| G: -5312.42844 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.85870 HOMO: -7.04231 LUMO: 1.79323 factor:1 | 1 (-1.06456) | 1 | 1 |
| G: -5312.42844 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.66534 HOMO: -6.68584 LUMO: 1.60275 factor:1 | 1 (-0.87120) | 1 | 1 |
| G: -5312.42844 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.54071 HOMO: -6.40556 LUMO: 1.45581 factor:1 | 1 (-0.74657) | -1 | -1 |
| G: -5312.42844 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.36441 HOMO: -6.94979 LUMO: 2.16603 factor:1 | 1 (-0.57027) | 1 | 1 |
| G: -5312.42844 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.77329 HOMO: -6.84911 LUMO: 1.89935 factor:1 | 1 (-0.97915) | 1 | 1 |
| G: -5312.42844 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.58389 HOMO: -6.22052 LUMO: 1.57282 factor:1 | 1 (-0.78976) | -1 | -1 |
| G: -5312.42844 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.74156 HOMO: -6.51168 LUMO: 2.10072 factor:1 | 1 (-0.94742) | -1 | -1 |
| G: -5312.42844 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.42620 HOMO: -7.03686 LUMO: 2.12249 factor:1 | 1 (-0.63207) | 1 | 1 |
| G: -5312.42844 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.33679 HOMO: -6.84094 LUMO: 1.63268 factor:1 | 1 (-0.54265) | 1 | 1 |
| G: -5312.42844 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.57853 HOMO: -6.75387 LUMO: 1.72248 factor:1 | 1 (-0.78440) | 1 | 1 |
| G: -5312.42844 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.45037 HOMO: -6.86271 LUMO: 1.68711 factor:1 | 1 (-0.65623) | 1 | 1 |
| G: -5312.42844 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.77092 HOMO: -6.84094 LUMO: 2.02997 factor:1 | 1 (-0.97678) | 1 | 1 |
| G: -5312.42844 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.41891 HOMO: -6.80557 LUMO: 2.02725 factor:1 | 1 (-0.62477) | 1 | 1 |
| G: -5312.42844 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.15923 HOMO: -6.38651 LUMO: 1.53472 factor:1 | 1 (-0.36510) | -1 | -1 |
| G: -5312.42844 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.44599 HOMO: -7.51306 LUMO: 0.28572 factor:1 | 1 (-0.65185) | -1 | -1 |
| G: -5312.42844 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.71337 HOMO: -6.97972 LUMO: -0.74287 factor:1 | 1 (-0.91923) | -1 | -1 |
| G: -5312.42844 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.48161 HOMO: -6.83822 LUMO: -0.65852 factor:1 | 1 (-0.68747) | -1 | -1 |
| G: -5312.42844 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.53709 HOMO: -6.71305 LUMO: -0.49525 factor:1 | 1 (-0.74295) | -1 | -1 |
| G: -5312.42844 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.56223 HOMO: -6.60692 LUMO: -0.22313 factor:1 | 1 (-0.76810) | -1 | -1 |
| G: -5312.42844 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.74335 HOMO: -7.20013 LUMO: 0.55239 factor:1 | 1 (-0.94921) | -1 | -1 |
| G: -5312.42844 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.69473 HOMO: -6.60420 LUMO: -0.28028 factor:1 | 1 (-0.90059) | -1 | -1 |
| G: -5312.42844 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.60112 HOMO: -6.69128 LUMO: -0.30477 factor:1 | 1 (-0.80698) | -1 | -1 |
| G: -5312.42844 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.88172 HOMO: -6.65591 LUMO: -0.25579 factor:1 | 1 (-1.08758) | -1 | -1 |
| G: -5312.42844 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.58727 HOMO: -6.69128 LUMO: 1.70888 factor:1 | 1 (-0.79313) | 1 | 1 |
| G: -5312.42844 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.75617 HOMO: -6.50080 LUMO: 1.87759 factor:1 | 1 (-0.96203) | -1 | -1 |
| G: -5312.42844 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.61453 HOMO: -6.85727 LUMO: 1.99187 factor:1 | 1 (-0.82040) | 1 | 1 |
| G: -5312.42844 HOMO: -6.56339 LUMO: 1.86126 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 (-0.74230) | 1 | 1 |
| G: -5312.42844 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.42729 HOMO: -6.64230 LUMO: 2.16058 factor:1 | 1 (-0.63315) | 1 | 1 |
| G: -5312.42844 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.44610 HOMO: -6.58788 LUMO: 2.10616 factor:1 | 1 (-0.65196) | 1 | 1 |
| G: -5312.42844 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.71035 HOMO: -7.01782 LUMO: 2.13609 factor:1 | 1 (-0.91621) | 1 | 1 |
| G: -5312.42844 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.81843 HOMO: -6.31304 LUMO: 2.31841 factor:1 | 1 (-1.02429) | -1 | -1 |
| G: -5312.42844 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.60485 HOMO: -6.94979 LUMO: 2.07895 factor:1 | 1 (-0.81071) | 1 | 1 |
| G: -5312.42844 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.39369 HOMO: -6.88992 LUMO: 2.28031 factor:1 | 1 (-0.59955) | 1 | 1 |
| G: -5312.42844 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.43410 HOMO: -6.66407 LUMO: 2.07623 factor:1 | 1 (-0.63996) | 1 | 1 |
| G: -5312.42844 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.32702 HOMO: -6.52529 LUMO: 1.70071 factor:1 | 1 (-0.53288) | -1 | -1 |
| G: -5312.42844 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.18974 HOMO: -6.58788 LUMO: 1.57282 factor:1 | 1 (-0.39560) | -1 | -1 |
| G: -5312.42844 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.70643 HOMO: -6.55250 LUMO: 1.95378 factor:1 | 1 (-0.91229) | -1 | -1 |
| G: -5312.42844 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.48514 HOMO: -6.24773 LUMO: 1.77962 factor:1 | 1 (-0.69101) | -1 | -1 |
| G: -5312.42844 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.14612 HOMO: -6.31304 LUMO: 2.18507 factor:1 | 1 (-0.35198) | -1 | -1 |
| G: -5312.42844 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.21548 HOMO: -6.18243 LUMO: 2.01636 factor:1 | 1 (-0.42134) | -1 | -1 |
| G: -5312.42844 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.52841 HOMO: -6.99877 LUMO: 2.14970 factor:1 | 1 (-0.73427) | 1 | 1 |
| G: -5312.42844 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.30457 HOMO: -6.72665 LUMO: 2.07079 factor:1 | 1 (-0.51043) | 1 | 1 |
| G: -5312.42844 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.37135 HOMO: -6.36202 LUMO: 2.17419 factor:1 | 1 (-0.57721) | -1 | -1 |
| G: -5312.42844 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11578.10940 HOMO: -6.78652 LUMO: 2.05718 factor:1 | 1 (-1.31526) | 1 | -1 |
| G: -5312.42844 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11578.39055 HOMO: -6.87360 LUMO: 2.34290 factor:1 | 1 (-1.59641) | 1 | 1 |
| G: -5312.42844 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11578.98925 HOMO: -6.62053 LUMO: 1.89391 factor:1 | 1 (-2.19512) | 1 | 1 |
| G: -5312.42844 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.70591 HOMO: -6.58788 LUMO: 1.83133 factor:1 | 1 (-0.91177) | 1 | 1 |
| G: -5312.42844 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11578.13473 HOMO: -7.08584 LUMO: 1.91568 factor:1 | 1 (-1.34060) | 1 | 1 |
| G: -5312.42844 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.74743 HOMO: -6.56883 LUMO: 1.81228 factor:1 | 1 (-0.95330) | 1 | 1 |
| G: -5312.42844 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11578.17299 HOMO: -6.66135 LUMO: 1.92384 factor:1 | 1 (-1.37886) | 1 | 1 |
| G: -5312.42844 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.99476 HOMO: -6.64502 LUMO: 2.15786 factor:1 | 1 (-1.20062) | 1 | 1 |
| G: -5312.42844 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11578.38946 HOMO: -6.71305 LUMO: 1.91840 factor:1 | 1 (-1.59532) | 1 | 1 |
| G: -5312.42844 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11578.93761 HOMO: -6.44094 LUMO: 1.74425 factor:1 | 1 (-2.14347) | -1 | -1 |
| G: -5312.42844 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11578.19879 HOMO: -6.51985 LUMO: 1.84221 factor:1 | 1 (-1.40465) | -1 | -1 |
| G: -5312.42844 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11578.45123 HOMO: -6.63414 LUMO: -0.24762 factor:1 | 1 (-1.65709) | -1 | -1 |
| G: -5312.42844 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11579.10898 HOMO: -6.60420 LUMO: -0.22585 factor:1 | 1 (-2.31485) | -1 | -1 |
| G: -5312.42844 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11578.98863 HOMO: -7.19741 LUMO: 0.58232 factor:1 | 1 (-2.19449) | -1 | -1 |
| G: -5312.42844 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.81339 HOMO: -6.77019 LUMO: -0.56872 factor:1 | 1 (-1.01926) | -1 | -1 |
| G: -5312.42844 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.96306 HOMO: -7.46136 LUMO: 0.28844 factor:1 | 1 (-1.16892) | -1 | -1 |
| G: -5312.42844 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11578.29947 HOMO: -6.60420 LUMO: -0.54151 factor:1 | 1 (-1.50533) | -1 | -1 |
| G: -5312.42844 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11578.18761 HOMO: -6.53890 LUMO: -0.46531 factor:1 | 1 (-1.39347) | -1 | -1 |
| G: -5312.42844 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.91223 HOMO: -6.81645 LUMO: -0.57144 factor:1 | 1 (-1.11809) | -1 | -1 |
| G: -5312.42844 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.69005 HOMO: -7.48041 LUMO: 0.28572 factor:1 | -1 (0.10408) | -1 | -1 |
| G: -5312.42844 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.85564 HOMO: -6.75659 LUMO: -0.45715 factor:1 | 1 (-0.06150) | -1 | -1 |
| G: -5312.42844 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.10307 HOMO: -6.66135 LUMO: -0.41906 factor:1 | 1 (-0.30893) | -1 | -1 |
| G: -5312.42844 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.79169 HOMO: -6.55794 LUMO: -0.27483 factor:1 | -1 (0.00245) | -1 | -1 |
| G: -5312.42844 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.60589 HOMO: -7.07496 LUMO: -0.63403 factor:1 | -1 (0.18825) | -1 | -1 |
| G: -5312.42844 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.64028 HOMO: -7.12394 LUMO: 0.53334 factor:1 | -1 (0.15385) | -1 | -1 |
| G: -5312.42844 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.65004 HOMO: -6.53617 LUMO: -0.25579 factor:1 | 1 (-0.85591) | -1 | -1 |
| G: -5312.42844 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11578.51580 HOMO: -6.50896 LUMO: -0.25034 factor:1 | 1 (-1.72166) | -1 | -1 |
| G: -5312.42844 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.97723 HOMO: -7.17564 LUMO: -0.68573 factor:1 | 1 (-1.18310) | -1 | -1 |
| G: -5312.42844 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.83108 HOMO: -6.53617 LUMO: -0.30749 factor:1 | 1 (-1.03694) | -1 | -1 |
| G: -5312.42844 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.58085 HOMO: -6.55522 LUMO: -0.30749 factor:1 | 1 (-0.78671) | -1 | -1 |
| G: -5312.42844 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.70308 HOMO: -7.05591 LUMO: -0.71022 factor:1 | 1 (-0.90894) | -1 | -1 |
| G: -5312.42844 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.59279 HOMO: -7.17564 LUMO: -0.69933 factor:1 | 1 (-0.79865) | -1 | -1 |
| G: -5312.42844 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.80050 HOMO: -6.78380 LUMO: -0.67756 factor:1 | 1 (-1.00636) | -1 | -1 |
| G: -5312.42844 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.65772 HOMO: -6.62325 LUMO: 2.02725 factor:1 | 1 (-0.86358) | 1 | 1 |
| G: -5312.42844 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.96877 HOMO: -6.63414 LUMO: 1.91296 factor:1 | 1 (-1.17463) | 1 | -1 |
| G: -5312.42844 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.76395 HOMO: -6.83278 LUMO: 1.65717 factor:1 | 1 (-0.96981) | 1 | 1 |
| G: -5312.42844 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11578.12815 HOMO: -6.66407 LUMO: 1.95650 factor:1 | 1 (-1.33401) | 1 | 1 |
| G: -5312.42844 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.97669 HOMO: -6.61237 LUMO: 2.11432 factor:1 | 1 (-1.18255) | 1 | 1 |
| G: -5312.42844 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11578.22407 HOMO: -6.62053 LUMO: 2.09256 factor:1 | 1 (-1.42993) | 1 | -1 |
| G: -5312.42844 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11578.80087 HOMO: -6.78652 LUMO: 2.13609 factor:1 | 1 (-2.00673) | 1 | 1 |
| G: -5312.42844 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11578.38970 HOMO: -6.94707 LUMO: 1.81772 factor:1 | 1 (-1.59557) | 1 | 1 |
| G: -5312.42844 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11578.15218 HOMO: -6.85183 LUMO: 2.12793 factor:1 | 1 (-1.35804) | 1 | 1 |
| G: -5312.42844 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.71168 HOMO: -6.81101 LUMO: 1.83949 factor:1 | 1 (-0.91754) | 1 | 1 |
| G: -5312.42844 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.95879 HOMO: -6.98788 LUMO: 2.16058 factor:1 | 1 (-1.16465) | 1 | 1 |
| G: -5312.42844 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.95217 HOMO: -6.62869 LUMO: 2.00820 factor:1 | 1 (-1.15803) | 1 | 1 |
| G: -5312.42844 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.82006 HOMO: -6.34025 LUMO: 2.25855 factor:1 | 1 (-1.02592) | -1 | -1 |
| G: -5312.42844 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.56789 HOMO: -6.01372 LUMO: 2.01636 factor:1 | 1 (-0.77376) | -1 | -1 |
| G: -5312.42844 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.91496 HOMO: -6.89264 LUMO: 2.27487 factor:1 | 1 (-0.12082) | 1 | 1 |
| G: -5312.42844 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.82407 HOMO: -6.53073 LUMO: 2.20684 factor:1 | 1 (-0.02993) | -1 | -1 |
| G: -5312.42844 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.93324 HOMO: -6.83278 LUMO: 1.53744 factor:1 | 1 (-0.13910) | -1 | -1 |
| G: -5312.42844 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.17480 HOMO: -6.41917 LUMO: 1.82316 factor:1 | 1 (-0.38066) | -1 | -1 |
| G: -5312.42844 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.12565 HOMO: -6.56339 LUMO: 1.63813 factor:1 | 1 (-0.33152) | -1 | -1 |
| G: -5312.42844 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.96225 HOMO: -6.88992 LUMO: 1.65173 factor:1 | 1 (-0.16811) | 1 | 1 |
| G: -5312.42844 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.93771 HOMO: -6.63141 LUMO: 1.92112 factor:1 | 1 (-0.14357) | 1 | 1 |
| G: -5312.42844 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.74475 HOMO: -6.83822 LUMO: 1.88847 factor:1 | -1 (0.04939) | 1 | 1 |
| G: -5312.42844 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.76276 HOMO: -6.84638 LUMO: 1.90480 factor:1 | -1 (0.03137) | 1 | 1 |
| G: -5312.42844 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.68878 HOMO: -6.82462 LUMO: 1.70888 factor:1 | -1 (0.10536) | 1 | 1 |
| G: -5312.42844 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.82366 HOMO: -6.82734 LUMO: 2.12521 factor:1 | 1 (-0.02952) | 1 | 1 |
| G: -5312.42844 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.95049 HOMO: -6.94435 LUMO: 1.87214 factor:1 | 1 (-0.15636) | 1 | 1 |
| G: -5312.42844 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.92440 HOMO: -6.98516 LUMO: 2.51433 factor:1 | 1 (-0.13026) | 1 | 1 |
| G: -5312.42844 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: 2.15514 factor:1 | 1 (-0.25998) | 1 | 1 |
| G: -5312.42844 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.09031 HOMO: -6.93618 LUMO: 2.54426 factor:1 | 1 (-0.29617) | 1 | 1 |
| G: -5312.42844 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.87694 HOMO: -6.28583 LUMO: 2.53610 factor:1 | 1 (-0.08280) | -1 | -1 |
| G: -5312.42844 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.82834 HOMO: -6.56883 LUMO: 1.94834 factor:1 | 1 (-0.03420) | 1 | 1 |
| G: -5312.42844 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.66026 HOMO: -7.08584 LUMO: 1.99187 factor:1 | -1 (0.13388) | 1 | 1 |
| G: -5312.42844 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.80815 HOMO: -6.19059 LUMO: 1.99732 factor:1 | 1 (-0.01401) | -1 | -1 |
| G: -5312.42844 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.68761 HOMO: -6.78108 LUMO: 2.03813 factor:1 | -1 (0.10653) | 1 | 1 |
| G: -5312.42844 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.85621 HOMO: -6.82189 LUMO: 1.77418 factor:1 | 1 (-0.06207) | 1 | 1 |
| G: -5312.42844 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.69539 HOMO: -6.45454 LUMO: 1.78779 factor:1 | -1 (0.09875) | -1 | -1 |
| G: -5312.42844 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.11999 HOMO: -6.84366 LUMO: 1.77690 factor:1 | 1 (-0.32586) | 1 | 1 |
| G: -5312.42844 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.89506 HOMO: -6.74026 LUMO: 1.67622 factor:1 | 1 (-0.10093) | 1 | 1 |
| G: -5312.42844 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.90440 HOMO: -6.76475 LUMO: 2.40277 factor:1 | 1 (-0.11026) | 1 | 1 |
| G: -5312.42844 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.75476 HOMO: -6.65863 LUMO: 1.86670 factor:1 | -1 (0.03937) | 1 | 1 |
| G: -5312.42844 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.67280 HOMO: -6.50080 LUMO: 1.93201 factor:1 | -1 (0.12134) | -1 | -1 |
| G: -5312.42844 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.55190 HOMO: -6.34842 LUMO: 1.70888 factor:1 | -1 (0.24224) | -1 | -1 |
| G: -5312.42844 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.70110 HOMO: -6.60692 LUMO: 2.20140 factor:1 | -1 (0.09304) | 1 | 1 |
| G: -5312.42844 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.94277 HOMO: -6.74026 LUMO: 2.14970 factor:1 | 1 (-0.14863) | 1 | 1 |
| G: -5312.42844 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11578.14483 HOMO: -6.63686 LUMO: 2.17419 factor:1 | 1 (-1.35069) | 1 | 1 |
| G: -5312.42844 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11579.07984 HOMO: -6.81917 LUMO: 2.10072 factor:1 | 1 (-2.28570) | 1 | -1 |
| G: -5312.42844 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11578.29335 HOMO: -6.92802 LUMO: 2.04358 factor:1 | 1 (-1.49921) | 1 | 1 |
| G: -5312.42844 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11578.20937 HOMO: -6.56067 LUMO: -0.47620 factor:1 | 1 (-1.41524) | -1 | -1 |
| G: -5312.42844 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.98635 HOMO: -6.56611 LUMO: -0.77008 factor:1 | 1 (-1.19221) | -1 | -1 |
| G: -5312.42844 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.75493 HOMO: -6.78380 LUMO: -0.64763 factor:1 | -1 (0.03921) | -1 | -1 |
| G: -5312.42844 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.73351 HOMO: -6.51985 LUMO: -0.24490 factor:1 | -1 (0.06063) | -1 | -1 |
| G: -5312.42844 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.96571 HOMO: -6.52529 LUMO: -0.27483 factor:1 | 1 (-0.17157) | -1 | -1 |
| G: -5312.42844 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.84187 HOMO: -7.10489 LUMO: -0.62586 factor:1 | 1 (-0.04773) | -1 | -1 |
| G: -5312.42844 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.59903 HOMO: -7.18108 LUMO: 0.48980 factor:1 | -1 (0.19511) | -1 | -1 |
| G: -5312.42844 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.50972 HOMO: -7.14299 LUMO: -0.63947 factor:1 | -1 (0.28441) | -1 | -1 |
| G: -5312.42844 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.69416 HOMO: -6.70761 LUMO: -0.54423 factor:1 | -1 (0.09997) | -1 | -1 |
| G: -5312.42844 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.87185 HOMO: -7.32258 LUMO: -1.03675 factor:1 | 1 (-0.07772) | -1 | -1 |
| G: -5312.42844 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.73758 HOMO: -6.65046 LUMO: -0.41361 factor:1 | 1 (-0.94345) | -1 | -1 |
| G: -5312.42844 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11578.44568 HOMO: -6.76475 LUMO: -0.60137 factor:1 | 1 (-1.65154) | -1 | -1 |
| G: -5312.42844 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.76953 HOMO: -6.77836 LUMO: -0.54423 factor:1 | 1 (-0.97539) | -1 | -1 |
| G: -5312.42844 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.97966 HOMO: -7.52395 LUMO: 0.26395 factor:1 | 1 (-1.18552) | -1 | -1 |
| G: -5312.42844 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.87266 HOMO: -6.93890 LUMO: -0.72382 factor:1 | 1 (-1.07852) | -1 | -1 |
| G: -5312.42844 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.59456 HOMO: -6.72938 LUMO: -0.47348 factor:1 | 1 (-0.80042) | -1 | -1 |
| G: -5312.42844 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.75707 HOMO: -6.66951 LUMO: -0.40817 factor:1 | 1 (-0.96293) | -1 | -1 |
| G: -5312.42844 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.92602 HOMO: -6.60420 LUMO: -0.19320 factor:1 | 1 (-1.13188) | -1 | -1 |
| G: -5312.42844 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.78575 HOMO: -6.67495 LUMO: -0.27211 factor:1 | 1 (-0.99161) | -1 | -1 |
| G: -5312.42844 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.54844 HOMO: -7.23823 LUMO: -0.62858 factor:1 | 1 (-0.75430) | -1 | -1 |
| G: -5312.42844 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11578.10545 HOMO: -7.27088 LUMO: 0.53334 factor:1 | 1 (-1.31132) | -1 | -1 |
| G: -5312.42844 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.93704 HOMO: -7.20013 LUMO: 0.59049 factor:1 | 1 (-1.14291) | -1 | -1 |
| G: -5312.42844 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11578.16984 HOMO: -6.60148 LUMO: -0.20953 factor:1 | 1 (-1.37570) | -1 | -1 |
| G: -5312.42844 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.91927 HOMO: -6.69400 LUMO: -0.51974 factor:1 | 1 (-1.12514) | -1 | -1 |
| G: -5312.42844 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11578.07949 HOMO: -7.40422 LUMO: -0.98777 factor:1 | 1 (-1.28536) | -1 | -1 |
| G: -5312.42844 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.76567 HOMO: -6.88176 LUMO: -0.71022 factor:1 | -1 (0.02846) | -1 | -1 |
| G: -5312.42844 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.54853 HOMO: -6.86271 LUMO: -0.59321 factor:1 | -1 (0.24561) | -1 | -1 |
| G: -5312.42844 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.85596 HOMO: -6.73754 LUMO: -0.55239 factor:1 | 1 (-0.06182) | -1 | -1 |
| G: -5312.42844 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.59808 HOMO: -6.71033 LUMO: 1.57010 factor:1 | -1 (0.19606) | -1 | -1 |
| G: -5312.42844 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.81115 HOMO: -6.69672 LUMO: 1.68711 factor:1 | 1 (-0.01701) | 1 | 1 |
| G: -5312.42844 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.78461 HOMO: -6.67495 LUMO: 2.03813 factor:1 | -1 (0.00952) | 1 | 1 |
| G: -5312.42844 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.56692 HOMO: -6.54434 LUMO: 1.83677 factor:1 | -1 (0.22722) | -1 | -1 |
| G: -5312.42844 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.54436 HOMO: -6.57155 LUMO: 1.77146 factor:1 | -1 (0.24977) | 1 | 1 |
| G: -5312.42844 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.34899 HOMO: -6.76747 LUMO: 1.87759 factor:1 | -1 (0.44515) | 1 | 1 |
| G: -5312.42844 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.72344 HOMO: -6.58243 LUMO: 1.61364 factor:1 | -1 (0.07070) | 1 | 1 |
| G: -5312.42844 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.74235 HOMO: -6.61781 LUMO: 2.13881 factor:1 | 1 (-0.94821) | 1 | 1 |
| G: -5312.42844 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.55516 HOMO: -6.62597 LUMO: 2.00276 factor:1 | 1 (-0.76102) | 1 | 1 |
| G: -5312.42844 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11578.59292 HOMO: -7.01237 LUMO: 1.95922 factor:1 | 1 (-1.79878) | 1 | 1 |
| G: -5312.42844 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.58553 HOMO: -7.03959 LUMO: 2.16875 factor:1 | 1 (-0.79139) | 1 | 1 |
| G: -5312.42844 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.82621 HOMO: -6.83278 LUMO: 1.91296 factor:1 | 1 (-1.03207) | 1 | 1 |
| G: -5312.42844 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.78539 HOMO: -6.40012 LUMO: 1.95650 factor:1 | 1 (-0.99126) | -1 | -1 |
| G: -5312.42844 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.81100 HOMO: -6.50080 LUMO: 1.73337 factor:1 | 1 (-1.01686) | -1 | -1 |
| G: -5312.42844 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.61336 HOMO: -6.95795 LUMO: 2.28848 factor:1 | 1 (-0.81923) | 1 | 1 |
| G: -5312.42844 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.80537 HOMO: -6.63686 LUMO: 2.20140 factor:1 | 1 (-1.01123) | 1 | -1 |
| G: -5312.42844 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.02780 HOMO: -6.57427 LUMO: 1.87214 factor:1 | 1 (-0.23366) | 1 | -1 |
| G: -5312.42844 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.89789 HOMO: -6.38379 LUMO: 2.32113 factor:1 | 1 (-0.10376) | -1 | -1 |
| G: -5312.42844 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.94946 HOMO: -6.63958 LUMO: 2.04902 factor:1 | 1 (-0.15532) | 1 | 1 |
| G: -5312.42844 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.06759 HOMO: -6.70216 LUMO: 1.93201 factor:1 | 1 (-0.27345) | 1 | 1 |
| G: -5312.42844 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.90641 HOMO: -6.80557 LUMO: 2.23678 factor:1 | 1 (-0.11227) | 1 | 1 |
| G: -5312.42844 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.71041 HOMO: -6.72938 LUMO: 2.28304 factor:1 | -1 (0.08373) | 1 | 1 |
| G: -5312.42844 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.81270 HOMO: -6.56067 LUMO: 1.66806 factor:1 | 1 (-0.01856) | -1 | -1 |
| G: -5312.42844 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.96054 HOMO: -6.95523 LUMO: 2.33474 factor:1 | 1 (-0.16640) | 1 | 1 |
| G: -5312.42844 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.21268 HOMO: -6.59876 LUMO: 2.30480 factor:1 | 1 (-0.41854) | 1 | 1 |
| G: -5312.42844 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.08187 HOMO: -6.87360 LUMO: 1.75786 factor:1 | 1 (-0.28773) | 1 | 1 |
| G: -5312.42844 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.20574 HOMO: -7.06408 LUMO: 1.99187 factor:1 | 1 (-0.41160) | 1 | 1 |
| G: -5312.42844 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.07199 HOMO: -6.95795 LUMO: 1.88847 factor:1 | 1 (-0.27786) | 1 | 1 |
| G: -5312.42844 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.04816 HOMO: -6.85455 LUMO: 1.63813 factor:1 | 1 (-0.25402) | 1 | 1 |
| G: -5312.42844 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.85226 HOMO: -7.09129 LUMO: 2.31569 factor:1 | 1 (-0.05812) | 1 | 1 |
| G: -5312.42844 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.98435 HOMO: -6.91441 LUMO: 1.68983 factor:1 | 1 (-0.19021) | 1 | 1 |
| G: -5312.42844 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.01730 HOMO: -6.89809 LUMO: 2.23678 factor:1 | 1 (-0.22316) | 1 | 1 |
| G: -5312.42844 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.18955 HOMO: -6.78652 LUMO: 1.98371 factor:1 | 1 (-0.39541) | 1 | -1 |
| G: -5312.42844 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.97814 HOMO: -6.94707 LUMO: 2.23678 factor:1 | 1 (-0.18400) | 1 | 1 |
| G: -5312.42844 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.21940 HOMO: -7.07224 LUMO: 2.13337 factor:1 | 1 (-0.42526) | 1 | 1 |
| G: -5312.42844 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.05120 HOMO: -6.94979 LUMO: 2.28031 factor:1 | 1 (-0.25707) | 1 | 1 |
| G: -5312.42844 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.80480 HOMO: -6.60965 LUMO: 2.20412 factor:1 | 1 (-0.01067) | 1 | 1 |
| G: -5312.42844 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.98315 HOMO: -6.87360 LUMO: 2.40277 factor:1 | 1 (-0.18901) | 1 | -1 |
| G: -5312.42844 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.86979 HOMO: -6.92802 LUMO: 1.89663 factor:1 | 1 (-0.07565) | 1 | -1 |
| G: -5312.42844 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.76970 HOMO: -6.88448 LUMO: 2.02725 factor:1 | -1 (0.02444) | 1 | 1 |
| G: -5312.42844 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.98927 HOMO: -6.69128 LUMO: 1.55105 factor:1 | 1 (-0.19513) | -1 | -1 |
| G: -5312.42844 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.84516 HOMO: -6.54978 LUMO: 1.93201 factor:1 | 1 (-0.05102) | -1 | -1 |
| G: -5312.42844 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.12816 HOMO: -6.19331 LUMO: 1.46941 factor:1 | 1 (-0.33402) | -1 | -1 |
| G: -5312.42844 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.92805 HOMO: -6.55794 LUMO: 1.89663 factor:1 | 1 (-0.13391) | -1 | -1 |
| G: -5312.42844 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.12729 HOMO: -6.07630 LUMO: 1.94289 factor:1 | 1 (-0.33315) | -1 | -1 |
| G: -5312.42844 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.93028 HOMO: -7.46408 LUMO: 0.31565 factor:1 | 1 (-0.13614) | -1 | -1 |
| G: -5312.42844 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.77710 HOMO: -6.63958 LUMO: -0.61770 factor:1 | -1 (0.01703) | -1 | -1 |
| G: -5312.42844 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.84151 HOMO: -6.81101 LUMO: -0.57960 factor:1 | 1 (-0.04738) | -1 | -1 |
| G: -5312.42844 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.59060 HOMO: -6.74298 LUMO: -0.57960 factor:1 | -1 (0.20354) | -1 | -1 |
| G: -5312.42844 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.63027 HOMO: -6.63686 LUMO: -0.42994 factor:1 | -1 (0.16387) | -1 | -1 |
| G: -5312.42844 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.60276 HOMO: -6.60965 LUMO: -0.41089 factor:1 | -1 (0.19138) | -1 | -1 |
| G: -5312.42844 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.47770 HOMO: -6.60692 LUMO: -0.80274 factor:1 | -1 (0.31644) | -1 | -1 |
| G: -5312.42844 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.97346 HOMO: -6.58788 LUMO: -0.78097 factor:1 | 1 (-0.17932) | -1 | -1 |
| G: -5312.42844 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.07588 HOMO: -6.67767 LUMO: -0.48436 factor:1 | 1 (-0.28175) | -1 | -1 |
| G: -5312.42844 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.02892 HOMO: -6.63141 LUMO: -0.40545 factor:1 | 1 (-0.23478) | -1 | -1 |
| G: -5312.42844 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.90965 HOMO: -6.62053 LUMO: -0.83811 factor:1 | 1 (-0.11551) | -1 | -1 |
| G: -5312.42844 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.13540 HOMO: -6.59604 LUMO: -0.35375 factor:1 | 1 (-0.34126) | -1 | -1 |
| G: -5312.42844 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.24680 HOMO: -6.34297 LUMO: -0.39729 factor:1 | 1 (-0.45266) | -1 | -1 |
| G: -5312.42844 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.13428 HOMO: -6.67223 LUMO: 1.97827 factor:1 | 1 (-0.34014) | 1 | 1 |
| G: -5312.42844 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.15844 HOMO: -6.40012 LUMO: 1.89935 factor:1 | 1 (-0.36431) | -1 | -1 |
| G: -5312.42844 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.02046 HOMO: -6.74842 LUMO: 1.97283 factor:1 | 1 (-0.22632) | 1 | -1 |
| G: -5312.42844 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.83944 HOMO: -6.76747 LUMO: 2.17147 factor:1 | 1 (-0.04531) | 1 | 1 |
| G: -5312.42844 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.77604 HOMO: -6.72121 LUMO: 1.55649 factor:1 | -1 (0.01810) | -1 | -1 |
| G: -5312.42844 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.79210 HOMO: -6.97700 LUMO: 2.04085 factor:1 | -1 (0.00204) | 1 | 1 |
| G: -5312.42844 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.98617 HOMO: -7.06680 LUMO: 2.04085 factor:1 | 1 (-0.19203) | 1 | -1 |
| G: -5312.42844 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.66085 HOMO: -7.09673 LUMO: 2.35106 factor:1 | 1 (-0.86671) | 1 | 1 |
| G: -5312.42844 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.42819 HOMO: -6.83006 LUMO: 2.14970 factor:1 | 1 (-0.63405) | 1 | 1 |
| G: -5312.42844 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.75987 HOMO: -6.72665 LUMO: 2.20140 factor:1 | 1 (-0.96573) | 1 | -1 |
| G: -5312.42844 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.91451 HOMO: -6.77291 LUMO: 2.34562 factor:1 | 1 (-1.12037) | 1 | -1 |
| G: -5312.42844 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.72196 HOMO: -6.73754 LUMO: 2.00276 factor:1 | 1 (-0.92783) | 1 | -1 |
| G: -5312.42844 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.96485 HOMO: -7.04231 LUMO: 1.92112 factor:1 | 1 (-1.17072) | 1 | -1 |
| G: -5312.42844 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.49037 HOMO: -6.83822 LUMO: 1.72248 factor:1 | 1 (-0.69623) | 1 | 1 |
| G: -5312.42844 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.46819 HOMO: -6.57971 LUMO: 2.16603 factor:1 | 1 (-0.67405) | 1 | -1 |
| G: -5312.42844 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.34155 HOMO: -6.80013 LUMO: 1.88575 factor:1 | 1 (-0.54741) | 1 | 1 |
| G: -5312.42844 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.64501 HOMO: -6.93618 LUMO: 2.18235 factor:1 | 1 (-0.85087) | 1 | 1 |
| G: -5312.42844 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.70632 HOMO: -6.54706 LUMO: 1.91024 factor:1 | 1 (-0.91218) | -1 | -1 |
| G: -5312.42844 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.79822 HOMO: -7.06952 LUMO: 2.18507 factor:1 | 1 (-0.00408) | 1 | 1 |
| G: -5312.42844 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.84396 HOMO: -7.05047 LUMO: 1.82044 factor:1 | 1 (-0.04982) | 1 | 1 |
| G: -5312.42844 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.08105 HOMO: -6.87632 LUMO: 1.92657 factor:1 | 1 (-0.28692) | 1 | 1 |
| G: -5312.42844 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.68439 HOMO: -6.58788 LUMO: 1.91568 factor:1 | -1 (0.10974) | 1 | -1 |
| G: -5312.42844 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.87164 HOMO: -7.17292 LUMO: 1.90752 factor:1 | 1 (-0.07750) | 1 | 1 |
| G: -5312.42844 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.73591 HOMO: -6.93890 LUMO: 1.80684 factor:1 | -1 (0.05823) | 1 | 1 |
| G: -5312.42844 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.89139 HOMO: -7.10761 LUMO: 2.20956 factor:1 | 1 (-0.09725) | 1 | 1 |
| G: -5312.42844 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.15583 HOMO: -6.85727 LUMO: 2.13609 factor:1 | 1 (-0.36169) | 1 | -1 |
| G: -5312.42844 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.85346 HOMO: -6.64502 LUMO: 1.38506 factor:1 | 1 (-0.05932) | -1 | -1 |
| G: -5312.42844 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.84862 HOMO: -6.87360 LUMO: 1.15648 factor:1 | 1 (-0.05448) | -1 | -1 |
| G: -5312.42844 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.71857 HOMO: -6.67223 LUMO: 2.07351 factor:1 | -1 (0.07557) | 1 | 1 |
| G: -5312.42844 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.41503 HOMO: -6.29671 LUMO: 2.43270 factor:1 | -1 (0.37911) | -1 | -1 |
| G: -5312.42844 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.74089 HOMO: -6.90897 LUMO: 2.28848 factor:1 | -1 (0.05325) | 1 | 1 |
| G: -5312.42844 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.96562 HOMO: -7.04231 LUMO: 1.70071 factor:1 | 1 (-0.17149) | 1 | 1 |
| G: -5312.42844 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.63555 HOMO: -6.69944 LUMO: 1.94834 factor:1 | -1 (0.15859) | 1 | 1 |
| G: -5312.42844 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.75743 HOMO: -6.56067 LUMO: 2.20956 factor:1 | -1 (0.03671) | -1 | -1 |
| G: -5312.42844 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.54842 HOMO: -6.65046 LUMO: 2.06807 factor:1 | -1 (0.24572) | 1 | -1 |
| G: -5312.42844 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.11017 HOMO: -7.08584 LUMO: 1.98915 factor:1 | 1 (-0.31603) | 1 | 1 |
| G: -5312.42844 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.75640 HOMO: -6.69400 LUMO: 2.09256 factor:1 | -1 (0.03774) | 1 | 1 |
| G: -5312.42844 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.62377 HOMO: -6.62869 LUMO: 2.16331 factor:1 | -1 (0.17037) | 1 | 1 |
| G: -5312.42844 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.77509 HOMO: -6.85183 LUMO: 2.16058 factor:1 | -1 (0.01905) | 1 | 1 |
| G: -5312.42844 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.97354 HOMO: -6.54706 LUMO: 1.92384 factor:1 | 1 (-0.17940) | -1 | -1 |
| G: -5312.42844 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.72023 HOMO: -6.84366 LUMO: 2.48984 factor:1 | -1 (0.07391) | 1 | 1 |
| G: -5312.42844 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.50423 HOMO: -6.77291 LUMO: 2.46263 factor:1 | -1 (0.28991) | 1 | 1 |
| G: -5312.42844 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.76668 HOMO: -7.01782 LUMO: 2.31025 factor:1 | -1 (0.02746) | 1 | 1 |
| G: -5312.42844 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.78328 HOMO: -6.94707 LUMO: 2.29664 factor:1 | -1 (0.01086) | 1 | 1 |
| G: -5312.42844 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.83596 HOMO: -6.64230 LUMO: 1.97283 factor:1 | 1 (-0.04182) | 1 | 1 |
| G: -5312.42844 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.87879 HOMO: -6.47359 LUMO: 2.20412 factor:1 | 1 (-0.08465) | -1 | -1 |
| G: -5312.42844 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.06726 HOMO: -6.90625 LUMO: 1.92384 factor:1 | 1 (-0.27312) | 1 | 1 |
| G: -5312.42844 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.90992 HOMO: -7.17020 LUMO: 2.06807 factor:1 | 1 (-0.11578) | 1 | 1 |
| G: -5312.42844 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.82649 HOMO: -6.65046 LUMO: 2.20956 factor:1 | 1 (-0.03235) | 1 | -1 |
| G: -5312.42844 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.70554 HOMO: -7.07496 LUMO: 1.82861 factor:1 | -1 (0.08860) | 1 | 1 |
| G: -5312.42844 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.90200 HOMO: -6.83006 LUMO: 2.14970 factor:1 | 1 (-0.10787) | 1 | -1 |
| G: -5312.42844 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.74407 HOMO: -6.92802 LUMO: 1.99187 factor:1 | -1 (0.05007) | 1 | 1 |
| G: -5312.42844 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.78516 HOMO: -6.69672 LUMO: 2.36739 factor:1 | -1 (0.00898) | 1 | -1 |
| G: -5312.42844 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.54807 HOMO: -7.13755 LUMO: 2.00276 factor:1 | -1 (0.24607) | 1 | 1 |
| G: -5312.42844 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.60782 HOMO: -6.92530 LUMO: 2.25582 factor:1 | -1 (0.18632) | 1 | 1 |
| G: -5312.42844 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.43008 HOMO: -6.77564 LUMO: 1.97827 factor:1 | -1 (0.36406) | 1 | 1 |
| G: -5312.42844 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.74780 HOMO: -6.87904 LUMO: 1.60003 factor:1 | -1 (0.04634) | 1 | 1 |
| G: -5312.42844 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.09861 HOMO: -6.62869 LUMO: 1.90480 factor:1 | 1 (-0.30447) | 1 | 1 |
| G: -5312.42844 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.96581 HOMO: -6.71033 LUMO: 1.54833 factor:1 | 1 (-0.17168) | -1 | -1 |
| G: -5312.42844 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.06669 HOMO: -6.74298 LUMO: 1.47486 factor:1 | 1 (-0.27255) | -1 | -1 |
| G: -5312.42844 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.95052 HOMO: -6.77019 LUMO: 1.90480 factor:1 | 1 (-0.15638) | 1 | 1 |
| G: -5312.42844 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.89381 HOMO: -6.70489 LUMO: 1.99459 factor:1 | 1 (-0.09968) | 1 | 1 |
| G: -5312.42844 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.75468 HOMO: -6.73482 LUMO: 2.08711 factor:1 | -1 (0.03946) | 1 | 1 |
| G: -5312.42844 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.78323 HOMO: -6.46543 LUMO: 1.73881 factor:1 | -1 (0.01091) | -1 | -1 |
| G: -5312.42844 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.71925 HOMO: -6.96067 LUMO: 2.26127 factor:1 | -1 (0.07489) | 1 | 1 |
| G: -5312.42844 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.99975 HOMO: -6.67767 LUMO: 2.10616 factor:1 | 1 (-0.20561) | 1 | 1 |
| G: -5312.42844 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.68366 HOMO: -6.28855 LUMO: 2.35923 factor:1 | -1 (0.11048) | -1 | -1 |
| G: -5312.42844 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.91482 HOMO: -6.80285 LUMO: 1.62724 factor:1 | 1 (-0.12068) | 1 | 1 |
| G: -5312.42844 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.63188 HOMO: -6.85455 LUMO: 2.23133 factor:1 | -1 (0.16226) | 1 | 1 |
| G: -5312.42844 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.78793 HOMO: -6.51713 LUMO: 2.33474 factor:1 | -1 (0.00620) | -1 | -1 |
| G: -5312.42844 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.48265 HOMO: -6.88176 LUMO: 2.15242 factor:1 | -1 (0.31149) | 1 | 1 |
| G: -5312.42844 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.77427 HOMO: -6.54434 LUMO: 2.32113 factor:1 | -1 (0.01986) | -1 | -1 |
| G: -5312.42844 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.60766 HOMO: -6.62597 LUMO: 2.24222 factor:1 | -1 (0.18648) | 1 | 1 |
| G: -5312.42844 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.65694 HOMO: -6.74570 LUMO: 2.19868 factor:1 | -1 (0.13720) | 1 | 1 |
| G: -5312.42844 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.39843 HOMO: -6.62869 LUMO: 1.98915 factor:1 | -1 (0.39571) | 1 | 1 |
| G: -5312.42844 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.97479 HOMO: -6.64502 LUMO: 2.13881 factor:1 | 1 (-0.18066) | 1 | 1 |
| G: -5312.42844 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.03743 HOMO: -6.95795 LUMO: 1.82316 factor:1 | 1 (-0.24330) | 1 | 1 |
| G: -5312.42844 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.13760 HOMO: -6.77291 LUMO: 1.36329 factor:1 | 1 (-0.34346) | -1 | -1 |
| G: -5312.42844 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.09050 HOMO: -6.45726 LUMO: 1.73064 factor:1 | 1 (-0.29636) | -1 | -1 |
| G: -5312.42844 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.11341 HOMO: -6.49264 LUMO: 1.77418 factor:1 | 1 (-0.31927) | -1 | -1 |
| G: -5312.42844 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.85264 HOMO: -6.60420 LUMO: 2.20956 factor:1 | 1 (-0.05850) | 1 | 1 |
| G: -5312.42844 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.86195 HOMO: -6.56067 LUMO: 2.05718 factor:1 | 1 (-0.06781) | -1 | -1 |
| G: -5312.42844 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.26843 HOMO: -6.62597 LUMO: 1.70343 factor:1 | 1 (-0.47429) | 1 | 1 |
| G: -5312.42844 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.09311 HOMO: -6.69400 LUMO: 2.16875 factor:1 | 1 (-0.29897) | 1 | 1 |
| G: -5312.42844 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: 2.11977 factor:1 | 1 (-0.37228) | 1 | 1 |
| G: -5312.42844 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.03765 HOMO: -6.92802 LUMO: 1.82044 factor:1 | 1 (-0.24351) | 1 | -1 |
| G: -5312.42844 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.96701 HOMO: -6.56339 LUMO: 2.30480 factor:1 | 1 (-0.17287) | -1 | -1 |
| G: -5312.42844 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.95469 HOMO: -6.63958 LUMO: 1.91024 factor:1 | 1 (-0.16055) | 1 | -1 |
| G: -5312.42844 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.96048 HOMO: -6.93074 LUMO: 2.05446 factor:1 | 1 (-0.16634) | 1 | 1 |
| G: -5312.42844 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.07602 HOMO: -6.61509 LUMO: 2.03813 factor:1 | 1 (-0.28188) | 1 | 1 |
| G: -5312.42844 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.20103 HOMO: -6.61237 LUMO: 1.91296 factor:1 | 1 (-0.40689) | 1 | -1 |
| G: -5312.42844 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.24808 HOMO: -6.86815 LUMO: 1.95378 factor:1 | 1 (-0.45394) | 1 | 1 |
| G: -5312.42844 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: 1.70888 factor:1 | 1 (-0.29617) | 1 | 1 |
| G: -5312.42844 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.04266 HOMO: -6.57971 LUMO: 2.20140 factor:1 | 1 (-0.24852) | 1 | -1 |
| G: -5312.42844 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.75539 HOMO: -6.41100 LUMO: 1.96738 factor:1 | -1 (0.03875) | -1 | -1 |
| G: -5312.42844 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.75144 HOMO: -6.90081 LUMO: 1.65989 factor:1 | -1 (0.04269) | 1 | 1 |
| G: -5312.42844 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.83623 HOMO: -6.68312 LUMO: 1.97827 factor:1 | 1 (-0.04210) | 1 | -1 |
| G: -5312.42844 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.10974 HOMO: -6.65318 LUMO: 2.10888 factor:1 | 1 (-0.31560) | 1 | -1 |
| G: -5312.42844 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.86965 HOMO: -6.62053 LUMO: 2.28848 factor:1 | 1 (-0.07551) | 1 | -1 |
| G: -5312.42844 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.16359 HOMO: -6.65863 LUMO: 2.29664 factor:1 | 1 (-0.36945) | 1 | -1 |
| G: -5312.42844 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.74208 HOMO: -6.63958 LUMO: 2.07623 factor:1 | -1 (0.05206) | 1 | -1 |
| G: -5312.42844 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.93556 HOMO: -6.58243 LUMO: 2.20684 factor:1 | 1 (-0.14142) | 1 | 1 |
| G: -5312.42844 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.76067 HOMO: -6.59332 LUMO: 2.05174 factor:1 | -1 (0.03347) | 1 | -1 |
| G: -5312.42844 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.54066 HOMO: -6.95251 LUMO: 2.20140 factor:1 | -1 (0.25347) | 1 | 1 |
| G: -5312.42844 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.68371 HOMO: -6.84638 LUMO: 2.39732 factor:1 | -1 (0.11042) | 1 | 1 |
| G: -5312.42844 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.86832 HOMO: -6.86815 LUMO: 2.47896 factor:1 | 1 (-0.07418) | 1 | 1 |
| G: -5312.42844 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.85022 HOMO: -7.00693 LUMO: 2.43270 factor:1 | 1 (-0.05608) | 1 | 1 |
| G: -5312.42844 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.12492 HOMO: -6.58788 LUMO: 2.30208 factor:1 | 1 (-0.33078) | 1 | 1 |
| G: -5312.42844 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.86192 HOMO: -6.63958 LUMO: 2.28031 factor:1 | 1 (-0.06778) | 1 | 1 |
| G: -5312.42844 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.96160 HOMO: -6.74570 LUMO: 2.28304 factor:1 | 1 (-0.16746) | 1 | 1 |
| G: -5312.42844 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.74148 HOMO: -6.78380 LUMO: 2.16331 factor:1 | -1 (0.05265) | 1 | 1 |
| G: -5312.42844 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.05752 HOMO: -6.52529 LUMO: 2.05718 factor:1 | 1 (-0.26338) | -1 | -1 |
| G: -5312.42844 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.20187 HOMO: -6.41644 LUMO: 1.65445 factor:1 | 1 (-0.40774) | -1 | -1 |
| G: -5312.42844 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.82102 HOMO: -6.34570 LUMO: 1.22451 factor:1 | 1 (-0.02688) | -1 | -1 |
| G: -5312.42844 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.64412 HOMO: -6.14433 LUMO: 1.85582 factor:1 | -1 (0.15002) | -1 | -1 |
| G: -5312.42844 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.94372 HOMO: -6.62053 LUMO: 1.92112 factor:1 | 1 (-0.14958) | 1 | -1 |
| G: -5312.42844 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.71166 HOMO: -6.63414 LUMO: 1.61908 factor:1 | -1 (0.08248) | 1 | 1 |
| G: -5312.42844 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.63095 HOMO: -6.75931 LUMO: 1.87214 factor:1 | -1 (0.16319) | 1 | 1 |
| G: -5312.42844 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.45688 HOMO: -6.55794 LUMO: 1.77418 factor:1 | -1 (0.33726) | -1 | -1 |
| G: -5312.42844 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.96328 HOMO: -6.52801 LUMO: 1.82044 factor:1 | 1 (-0.16915) | -1 | -1 |
| G: -5312.42844 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.91428 HOMO: -6.77564 LUMO: 1.97827 factor:1 | 1 (-0.12014) | 1 | 1 |
| G: -5312.42844 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.16329 HOMO: -6.93890 LUMO: 1.81228 factor:1 | 1 (-0.36915) | 1 | 1 |
| G: -5312.42844 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.81452 HOMO: -6.85455 LUMO: 1.75513 factor:1 | 1 (-0.02038) | 1 | 1 |
| G: -5312.42844 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.68905 HOMO: -6.86815 LUMO: 1.64629 factor:1 | -1 (0.10509) | 1 | 1 |
| G: -5312.42844 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.73563 HOMO: -6.98516 LUMO: 1.84765 factor:1 | -1 (0.05850) | 1 | 1 |
| G: -5312.42844 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.96845 HOMO: -6.04637 LUMO: 1.94017 factor:1 | 1 (-0.17432) | -1 | -1 |
| G: -5312.42844 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.71142 HOMO: -6.86271 LUMO: 2.11977 factor:1 | -1 (0.08272) | 1 | -1 |
| G: -5312.42844 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.72592 HOMO: -6.72938 LUMO: 2.11160 factor:1 | -1 (0.06822) | 1 | -1 |
| G: -5312.42844 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.52129 HOMO: -7.01782 LUMO: 2.13609 factor:1 | -1 (0.27285) | 1 | 1 |
| G: -5312.42844 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.59177 HOMO: -6.18515 LUMO: 2.04630 factor:1 | -1 (0.20237) | -1 | -1 |
| G: -5312.42844 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.54140 HOMO: -6.60965 LUMO: 2.17147 factor:1 | -1 (0.25274) | 1 | -1 |
| G: -5312.42844 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.32188 HOMO: -6.87360 LUMO: 2.35378 factor:1 | -1 (0.47225) | 1 | 1 |
| G: -5312.42844 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.75631 HOMO: -6.72938 LUMO: 2.20140 factor:1 | -1 (0.03782) | 1 | -1 |
| G: -5312.42844 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.63870 HOMO: -6.88448 LUMO: 2.54154 factor:1 | 1 (-0.84456) | 1 | -1 |
| G: -5312.42844 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.80153 HOMO: -6.87087 LUMO: 2.16058 factor:1 | 1 (-1.00739) | 1 | 1 |
| G: -5312.42844 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.67432 HOMO: -7.11306 LUMO: 2.04085 factor:1 | 1 (-0.88018) | 1 | 1 |
| G: -5312.42844 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.73644 HOMO: -6.66951 LUMO: 1.68438 factor:1 | 1 (-0.94230) | 1 | 1 |
| G: -5312.42844 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.96877 HOMO: -7.08312 LUMO: 2.19324 factor:1 | 1 (-1.17463) | 1 | 1 |
| G: -5312.42844 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.95876 HOMO: -6.69128 LUMO: 2.13881 factor:1 | 1 (-1.16462) | 1 | -1 |
| G: -5312.42844 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.90872 HOMO: -6.80285 LUMO: 2.16603 factor:1 | 1 (-1.11458) | 1 | 1 |
| G: -5312.42844 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.92774 HOMO: -6.82189 LUMO: 2.46807 factor:1 | 1 (-1.13360) | 1 | 1 |
| G: -5312.42844 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.65769 HOMO: -6.78652 LUMO: 2.12521 factor:1 | 1 (-0.86355) | 1 | 1 |
| G: -5312.42844 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.63043 HOMO: -6.47903 LUMO: 1.70071 factor:1 | 1 (-0.83629) | -1 | -1 |
| G: -5312.42844 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.45026 HOMO: -6.37019 LUMO: 1.24356 factor:1 | 1 (-0.65612) | -1 | -1 |
| G: -5312.42844 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.56498 HOMO: -6.69400 LUMO: 1.67350 factor:1 | 1 (-0.77084) | 1 | 1 |
| G: -5312.42844 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.49097 HOMO: -7.51851 LUMO: 0.27756 factor:1 | 1 (-0.69683) | -1 | -1 |
| G: -5312.42844 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.48065 HOMO: -6.95795 LUMO: -0.72110 factor:1 | 1 (-0.68652) | -1 | -1 |
| G: -5312.42844 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.65290 HOMO: -6.88720 LUMO: -0.67484 factor:1 | 1 (-0.85876) | -1 | -1 |
| G: -5312.42844 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.98152 HOMO: -6.83550 LUMO: -0.57144 factor:1 | 1 (-0.18738) | -1 | -1 |
| G: -5312.42844 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.05708 HOMO: -6.80285 LUMO: -0.57144 factor:1 | 1 (-0.26294) | -1 | -1 |
| G: -5312.42844 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.11439 HOMO: -6.76475 LUMO: -0.53062 factor:1 | 1 (-0.32025) | -1 | -1 |
| G: -5312.42844 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.17559 HOMO: -6.66951 LUMO: 1.74969 factor:1 | 1 (-0.38145) | 1 | 1 |
| G: -5312.42844 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.18280 HOMO: -6.53345 LUMO: 1.89935 factor:1 | 1 (-0.38866) | -1 | -1 |
| G: -5312.42844 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.11270 HOMO: -6.65046 LUMO: 2.01364 factor:1 | 1 (-0.31856) | 1 | -1 |
| G: -5312.42844 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.90410 HOMO: -6.64230 LUMO: 2.11977 factor:1 | 1 (-0.10996) | 1 | -1 |
| G: -5312.42844 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.87038 HOMO: -6.44910 LUMO: 2.13337 factor:1 | 1 (-0.07625) | -1 | -1 |
| G: -5312.42844 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.75283 HOMO: -7.05591 LUMO: 1.98915 factor:1 | -1 (0.04131) | 1 | -1 |
| G: -5312.42844 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.90707 HOMO: -7.02326 LUMO: 2.49256 factor:1 | 1 (-0.11293) | 1 | 1 |
| G: -5312.42844 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.67103 HOMO: -6.32937 LUMO: 2.51161 factor:1 | -1 (0.12310) | -1 | -1 |
| G: -5312.42844 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.89659 HOMO: -6.96067 LUMO: 2.20140 factor:1 | 1 (-0.10245) | 1 | 1 |
| G: -5312.42844 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.69893 HOMO: -6.97972 LUMO: 2.55243 factor:1 | -1 (0.09521) | 1 | 1 |
| G: -5312.42844 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.93077 HOMO: -6.72665 LUMO: 2.46535 factor:1 | 1 (-0.13663) | 1 | 1 |
| G: -5312.42844 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.89904 HOMO: -6.41917 LUMO: 2.35106 factor:1 | 1 (-0.10490) | -1 | -1 |
| G: -5312.42844 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.77642 HOMO: -6.75114 LUMO: 2.32929 factor:1 | -1 (0.01771) | 1 | 1 |
| G: -5312.42844 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.86100 HOMO: -6.91713 LUMO: 2.27215 factor:1 | 1 (-0.06686) | 1 | 1 |
| G: -5312.42844 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.59930 HOMO: -6.54978 LUMO: 2.00276 factor:1 | -1 (0.19483) | -1 | -1 |
| G: -5312.42844 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.92663 HOMO: -6.62325 LUMO: 2.05990 factor:1 | 1 (-0.13249) | 1 | 1 |
| G: -5312.42844 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.68611 HOMO: -6.86271 LUMO: 2.14970 factor:1 | -1 (0.10803) | 1 | 1 |
| G: -5312.42844 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.55683 HOMO: -6.77564 LUMO: 2.25855 factor:1 | -1 (0.23731) | 1 | -1 |
| G: -5312.42844 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.51397 HOMO: -6.71305 LUMO: 1.94561 factor:1 | -1 (0.28017) | 1 | -1 |
| G: -5312.42844 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.76355 HOMO: -6.75659 LUMO: 1.94561 factor:1 | -1 (0.03059) | 1 | -1 |
| G: -5312.42844 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.57638 HOMO: -6.94979 LUMO: 2.33474 factor:1 | 1 (-0.78225) | 1 | -1 |
| G: -5312.42844 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.40958 HOMO: -6.85727 LUMO: 2.50345 factor:1 | 1 (-0.61544) | 1 | -1 |
| G: -5312.42844 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.54188 HOMO: -6.87360 LUMO: 2.43270 factor:1 | 1 (-0.74774) | 1 | -1 |
| G: -5312.42844 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.58384 HOMO: -6.57427 LUMO: 2.46807 factor:1 | 1 (-0.78970) | 1 | -1 |
| G: -5312.42844 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.70945 HOMO: -7.16204 LUMO: 2.15242 factor:1 | 1 (-0.91531) | 1 | 1 |
| G: -5312.42844 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.77786 HOMO: -6.62869 LUMO: 2.11432 factor:1 | 1 (-0.98372) | 1 | -1 |
| G: -5312.42844 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.55861 HOMO: -7.05591 LUMO: 2.26671 factor:1 | 1 (-0.76448) | 1 | -1 |
| G: -5312.42844 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.61418 HOMO: -7.13483 LUMO: 1.47758 factor:1 | 1 (-0.82004) | -1 | -1 |
| G: -5312.42844 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.50438 HOMO: -6.72938 LUMO: 1.57282 factor:1 | 1 (-0.71024) | -1 | -1 |
| G: -5312.42844 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.91176 HOMO: -6.17426 LUMO: 1.81228 factor:1 | 1 (-1.11763) | -1 | -1 |
| G: -5312.42844 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.48765 HOMO: -6.65318 LUMO: 1.93473 factor:1 | 1 (-0.69351) | 1 | -1 |
| G: -5312.42844 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.36862 HOMO: -6.18515 LUMO: 2.01364 factor:1 | 1 (-0.57449) | -1 | -1 |
| G: -5312.42844 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.25153 HOMO: -7.05591 LUMO: 2.13337 factor:1 | 1 (-0.45740) | 1 | 1 |
| G: -5312.42844 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.34509 HOMO: -6.90897 LUMO: 2.29664 factor:1 | 1 (-0.55095) | 1 | -1 |
| G: -5312.42844 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.64632 HOMO: -7.11034 LUMO: 2.17147 factor:1 | 1 (-0.85218) | 1 | 1 |
| G: -5312.42844 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.79182 HOMO: -6.82734 LUMO: 2.26671 factor:1 | 1 (-0.99768) | 1 | 1 |
| G: -5312.42844 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.57162 HOMO: -6.34842 LUMO: 2.34562 factor:1 | 1 (-0.77748) | -1 | -1 |
| G: -5312.42844 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.62871 HOMO: -6.62053 LUMO: 2.22861 factor:1 | 1 (-0.83457) | 1 | -1 |
| G: -5312.42844 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.87715 HOMO: -6.80557 LUMO: 2.07079 factor:1 | 1 (-1.08301) | 1 | -1 |
| G: -5312.42844 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.87813 HOMO: -6.60692 LUMO: 2.46263 factor:1 | 1 (-1.08399) | 1 | -1 |
| G: -5312.42844 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.57652 HOMO: -7.02054 LUMO: 2.08711 factor:1 | 1 (-0.78238) | 1 | -1 |
| G: -5312.42844 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.59940 HOMO: -6.78652 LUMO: 2.02453 factor:1 | 1 (-0.80527) | 1 | 1 |
| G: -5312.42844 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.48025 HOMO: -6.51168 LUMO: 2.06534 factor:1 | 1 (-0.68611) | -1 | -1 |
| G: -5312.42844 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.39891 HOMO: -6.50080 LUMO: 2.01636 factor:1 | 1 (-0.60477) | -1 | -1 |
| G: -5312.42844 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.41015 HOMO: -6.54434 LUMO: 1.84493 factor:1 | 1 (-0.61601) | -1 | -1 |
| G: -5312.42844 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.72392 HOMO: -6.47087 LUMO: 1.76330 factor:1 | 1 (-0.92979) | -1 | -1 |
| G: -5312.42844 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.55203 HOMO: -6.78924 LUMO: 2.39460 factor:1 | 1 (-0.75789) | 1 | 1 |
| G: -5312.42844 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.55497 HOMO: -6.59876 LUMO: 1.84493 factor:1 | 1 (-0.76083) | 1 | 1 |
| G: -5312.42844 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11578.15727 HOMO: -6.41644 LUMO: 2.05174 factor:1 | 1 (-1.36313) | -1 | -1 |
| G: -5312.42844 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11578.38769 HOMO: -6.52257 LUMO: 2.11160 factor:1 | 1 (-1.59355) | -1 | -1 |
| G: -5312.42844 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11578.98297 HOMO: -6.90897 LUMO: 2.34018 factor:1 | 1 (-2.18883) | 1 | 1 |
| G: -5312.42844 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.97255 HOMO: -6.97428 LUMO: 1.86126 factor:1 | 1 (-1.17842) | 1 | 1 |
| G: -5312.42844 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.96265 HOMO: -7.13483 LUMO: 2.14698 factor:1 | 1 (-1.16851) | 1 | -1 |
| G: -5312.42844 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11578.18861 HOMO: -7.16748 LUMO: 2.31841 factor:1 | 1 (-1.39447) | 1 | 1 |
| G: -5312.42844 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.99873 HOMO: -6.87087 LUMO: 2.38916 factor:1 | 1 (-1.20459) | 1 | -1 |
| G: -5312.42844 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.96820 HOMO: -6.93074 LUMO: 2.42181 factor:1 | 1 (-1.17406) | 1 | -1 |
| G: -5312.42844 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11578.19425 HOMO: -6.90081 LUMO: 2.00276 factor:1 | 1 (-1.40011) | 1 | -1 |
| G: -5312.42844 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.83141 HOMO: -6.99333 LUMO: 2.03541 factor:1 | 1 (-1.03727) | 1 | 1 |
| G: -5312.42844 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11578.98033 HOMO: -6.89264 LUMO: 1.57554 factor:1 | 1 (-2.18619) | -1 | -1 |
| G: -5312.42844 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11578.98218 HOMO: -6.48175 LUMO: 1.85854 factor:1 | 1 (-2.18804) | -1 | -1 |
| G: -5312.42844 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.79497 HOMO: -6.69400 LUMO: 1.62452 factor:1 | 1 (-1.00083) | 1 | 1 |
| G: -5312.42844 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11578.00496 HOMO: -6.50896 LUMO: 1.88303 factor:1 | 1 (-1.21083) | -1 | -1 |
| G: -5312.42844 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.93108 HOMO: -6.60420 LUMO: 2.05990 factor:1 | 1 (-1.13695) | 1 | 1 |
| G: -5312.42844 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.82882 HOMO: -7.14299 LUMO: 2.07351 factor:1 | 1 (-1.03469) | 1 | 1 |
| G: -5312.42844 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.58974 HOMO: -7.06408 LUMO: 1.81228 factor:1 | 1 (-0.79561) | 1 | 1 |
| G: -5312.42844 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11578.11101 HOMO: -6.67495 LUMO: 1.79595 factor:1 | 1 (-1.31687) | 1 | 1 |
| G: -5312.42844 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11578.38206 HOMO: -6.45182 LUMO: 2.15786 factor:1 | 1 (-1.58792) | -1 | -1 |
| G: -5312.42844 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11578.12611 HOMO: -6.93346 LUMO: 2.45719 factor:1 | 1 (-1.33197) | 1 | 1 |
| G: -5312.42844 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11578.10246 HOMO: -6.50080 LUMO: 2.08167 factor:1 | 1 (-1.30832) | -1 | -1 |
| G: -5312.42844 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.89930 HOMO: -6.83550 LUMO: -0.67484 factor:1 | 1 (-1.10516) | -1 | -1 |
| G: -5312.42844 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.80412 HOMO: -7.04231 LUMO: 0.54151 factor:1 | 1 (-0.00999) | -1 | -1 |
| G: -5312.42844 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: 1.91296 factor:1 | 1 (-0.04101) | -1 | -1 |
| G: -5312.42844 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.02075 HOMO: -7.35796 LUMO: -1.04220 factor:1 | 1 (-0.22662) | -1 | -1 |
| G: -5312.42844 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.78886 HOMO: -6.62597 LUMO: -0.44082 factor:1 | -1 (0.00528) | -1 | -1 |
| G: -5312.42844 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.73950 HOMO: -6.45182 LUMO: -0.20409 factor:1 | -1 (0.05464) | -1 | -1 |
| G: -5312.42844 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.80244 HOMO: -6.51168 LUMO: -0.23130 factor:1 | 1 (-0.00830) | -1 | -1 |
| G: -5312.42844 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.59253 HOMO: -7.14027 LUMO: 0.49797 factor:1 | -1 (0.20161) | -1 | -1 |
| G: -5312.42844 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.69710 HOMO: -7.55660 LUMO: 0.24762 factor:1 | -1 (0.09704) | -1 | -1 |
| G: -5312.42844 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.88628 HOMO: -6.88992 LUMO: -0.64763 factor:1 | 1 (-0.09214) | -1 | -1 |
| G: -5312.42844 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.77851 HOMO: -6.72665 LUMO: -0.45987 factor:1 | 1 (-0.98437) | -1 | -1 |
| G: -5312.42844 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11578.60606 HOMO: -6.72121 LUMO: -0.58232 factor:1 | 1 (-1.81192) | -1 | -1 |
| G: -5312.42844 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.94219 HOMO: -7.26816 LUMO: 0.32926 factor:1 | 1 (-1.14805) | -1 | -1 |
| G: -5312.42844 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.83549 HOMO: -6.57155 LUMO: -0.53606 factor:1 | 1 (-1.04135) | -1 | -1 |
| G: -5312.42844 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.77712 HOMO: -6.50896 LUMO: -0.43810 factor:1 | 1 (-0.98298) | -1 | -1 |
| G: -5312.42844 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.57110 HOMO: -6.73210 LUMO: -0.51430 factor:1 | 1 (-0.77697) | -1 | -1 |
| G: -5312.42844 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.80442 HOMO: -6.77019 LUMO: -0.62858 factor:1 | 1 (-1.01028) | -1 | -1 |
| G: -5312.42844 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.61530 HOMO: -6.82462 LUMO: -0.67484 factor:1 | 1 (-0.82116) | -1 | -1 |
| G: -5312.42844 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.80771 HOMO: -6.79740 LUMO: -0.55511 factor:1 | 1 (-1.01357) | -1 | -1 |
| G: -5312.42844 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.65108 HOMO: -6.79740 LUMO: -0.67756 factor:1 | 1 (-0.85694) | -1 | -1 |
| G: -5312.42844 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.80096 HOMO: -6.75114 LUMO: -0.55239 factor:1 | 1 (-1.00682) | -1 | -1 |
| G: -5312.42844 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.76194 HOMO: -6.49536 LUMO: -0.25307 factor:1 | 1 (-0.96780) | -1 | -1 |
| G: -5312.42844 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.88070 HOMO: -6.48992 LUMO: -0.25034 factor:1 | 1 (-0.08656) | -1 | -1 |
| G: -5312.42844 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.90424 HOMO: -6.52801 LUMO: -0.28028 factor:1 | 1 (-0.11010) | -1 | -1 |
| G: -5312.42844 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.00598 HOMO: -7.22462 LUMO: 0.52518 factor:1 | 1 (-0.21184) | -1 | -1 |
| G: -5312.42844 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.12816 HOMO: -6.59332 LUMO: -0.27211 factor:1 | 1 (-0.33402) | -1 | -1 |
| G: -5312.42844 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.02026 HOMO: -6.57427 LUMO: -0.16871 factor:1 | 1 (-0.22613) | -1 | -1 |
| G: -5312.42844 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.92772 HOMO: -6.71033 LUMO: 1.59187 factor:1 | 1 (-0.13358) | -1 | -1 |
| G: -5312.42844 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.90870 HOMO: -6.72121 LUMO: 2.00004 factor:1 | 1 (-0.11456) | -1 | -1 |
| G: -5312.42844 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.04040 HOMO: -6.61509 LUMO: 1.55921 factor:1 | 1 (-0.24626) | -1 | -1 |
| G: -5312.42844 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.96747 HOMO: -6.55250 LUMO: 1.73064 factor:1 | 1 (-0.17334) | -1 | -1 |
| G: -5312.42844 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.68956 HOMO: -6.66135 LUMO: 2.02181 factor:1 | -1 (0.10457) | -1 | -1 |
| G: -5312.42844 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.93128 HOMO: -6.84911 LUMO: 1.98099 factor:1 | 1 (-0.13715) | -1 | -1 |
| G: -5312.42844 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.76001 HOMO: -6.66679 LUMO: 1.98371 factor:1 | -1 (0.03412) | -1 | -1 |
| G: -5312.42844 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.96421 HOMO: -6.67495 LUMO: 2.04085 factor:1 | 1 (-0.17007) | -1 | -1 |
| G: -5312.42844 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.01020 HOMO: -6.89809 LUMO: 1.95106 factor:1 | 1 (-0.21606) | -1 | -1 |
| G: -5312.42844 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.77836 HOMO: -6.50352 LUMO: 1.88847 factor:1 | -1 (0.01578) | -1 | -1 |
| G: -5312.42844 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.00339 HOMO: -6.93618 LUMO: 2.00004 factor:1 | 1 (-0.20926) | -1 | -1 |
| G: -5312.42844 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.81721 HOMO: -6.50896 LUMO: 1.73609 factor:1 | 1 (-0.02308) | -1 | -1 |
| G: -5312.42844 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.98712 HOMO: -6.69672 LUMO: 2.37283 factor:1 | 1 (-0.19298) | -1 | -1 |
| G: -5312.42844 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.77871 HOMO: -6.65591 LUMO: 2.20684 factor:1 | -1 (0.01543) | -1 | -1 |
| G: -5312.42844 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.09684 HOMO: -6.23957 LUMO: 1.78507 factor:1 | 1 (-0.30270) | -1 | -1 |
| G: -5312.42844 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.80837 HOMO: -6.35114 LUMO: 1.92112 factor:1 | 1 (-0.01423) | -1 | -1 |
| G: -5312.42844 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.56178 HOMO: -6.53617 LUMO: 1.75241 factor:1 | -1 (0.23236) | -1 | -1 |
| G: -5312.42844 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.81928 HOMO: -6.60420 LUMO: 1.78779 factor:1 | 1 (-0.02514) | -1 | -1 |
| G: -5312.42844 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.04212 HOMO: -7.40422 LUMO: -0.97145 factor:1 | 1 (-0.24798) | -1 | -1 |
| G: -5312.42844 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.84208 HOMO: -6.80013 LUMO: -0.69117 factor:1 | 1 (-0.04795) | -1 | -1 |
| G: -5312.42844 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.93322 HOMO: -6.68040 LUMO: -0.47076 factor:1 | 1 (-0.13908) | -1 | -1 |
| G: -5312.42844 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.72227 HOMO: -7.20285 LUMO: -0.66124 factor:1 | -1 (0.07187) | -1 | -1 |
| G: -5312.42844 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.04337 HOMO: -6.82734 LUMO: -0.60137 factor:1 | 1 (-0.24923) | -1 | -1 |
| G: -5312.42844 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.83278 HOMO: -7.18653 LUMO: 0.59321 factor:1 | 1 (-0.03864) | -1 | -1 |
| G: -5312.42844 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.79207 HOMO: -7.29265 LUMO: 0.48164 factor:1 | -1 (0.00207) | -1 | -1 |
| G: -5312.42844 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.51941 HOMO: -6.63414 LUMO: -0.25034 factor:1 | -1 (0.27473) | -1 | -1 |
| G: -5312.42844 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.88617 HOMO: -7.20285 LUMO: 0.53879 factor:1 | 1 (-0.09203) | -1 | -1 |
| G: -5312.42844 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.62926 HOMO: -6.46815 LUMO: -0.21769 factor:1 | -1 (0.16487) | -1 | -1 |
| G: -5312.42844 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.44537 HOMO: -6.57971 LUMO: -0.18776 factor:1 | -1 (0.34877) | -1 | -1 |
| G: -5312.42844 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.64423 HOMO: -6.90897 LUMO: 1.91296 factor:1 | -1 (0.14991) | -1 | -1 |
| G: -5312.42844 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.80597 HOMO: -6.67495 LUMO: 2.04358 factor:1 | 1 (-0.01184) | -1 | -1 |
| G: -5312.42844 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.78347 HOMO: -6.94162 LUMO: 1.73881 factor:1 | -1 (0.01067) | -1 | -1 |
| G: -5312.42844 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.83830 HOMO: -6.73482 LUMO: 1.95922 factor:1 | 1 (-0.04416) | -1 | -1 |
| G: -5312.42844 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.88540 HOMO: -6.70489 LUMO: 2.04358 factor:1 | 1 (-0.09127) | -1 | -1 |
| G: -5312.42844 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.79493 HOMO: -7.04231 LUMO: 1.79323 factor:1 | 1 (-0.00079) | -1 | -1 |
| G: -5312.42844 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.75939 HOMO: -6.68584 LUMO: 1.60275 factor:1 | -1 (0.03475) | -1 | -1 |
| G: -5312.42844 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.79498 HOMO: -6.40556 LUMO: 1.45581 factor:1 | 1 (-0.00084) | -1 | -1 |
| G: -5312.42844 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.94500 HOMO: -6.94979 LUMO: 2.16603 factor:1 | 1 (-0.15086) | -1 | -1 |
| G: -5312.42844 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.10780 HOMO: -6.84911 LUMO: 1.89935 factor:1 | 1 (-0.31367) | -1 | -1 |
| G: -5312.42844 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.96911 HOMO: -6.22052 LUMO: 1.57282 factor:1 | 1 (-0.17497) | -1 | -1 |
| G: -5312.42844 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.01485 HOMO: -6.51168 LUMO: 2.10072 factor:1 | 1 (-0.22071) | -1 | -1 |
| G: -5312.42844 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.94728 HOMO: -7.03686 LUMO: 2.12249 factor:1 | 1 (-0.15315) | -1 | -1 |
| G: -5312.42844 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.91156 HOMO: -6.84094 LUMO: 1.63268 factor:1 | 1 (-0.11742) | -1 | -1 |
| G: -5312.42844 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.79046 HOMO: -6.75387 LUMO: 1.72248 factor:1 | -1 (0.00367) | -1 | -1 |
| G: -5312.42844 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.98707 HOMO: -6.86271 LUMO: 1.68711 factor:1 | 1 (-0.19293) | -1 | -1 |
| G: -5312.42844 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.87191 HOMO: -6.84094 LUMO: 2.02997 factor:1 | 1 (-0.07777) | -1 | -1 |
| G: -5312.42844 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.15814 HOMO: -6.80557 LUMO: 2.02725 factor:1 | 1 (-0.36401) | -1 | -1 |
| G: -5312.42844 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.97226 HOMO: -6.38651 LUMO: 1.53472 factor:1 | 1 (-0.17813) | -1 | -1 |
| G: -5312.42844 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.93123 HOMO: -7.51306 LUMO: 0.28572 factor:1 | 1 (-0.13709) | -1 | -1 |
| G: -5312.42844 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.89789 HOMO: -6.97972 LUMO: -0.74287 factor:1 | 1 (-0.10376) | -1 | -1 |
| G: -5312.42844 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.04990 HOMO: -6.83822 LUMO: -0.65852 factor:1 | 1 (-0.25576) | -1 | -1 |
| G: -5312.42844 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.78608 HOMO: -6.71305 LUMO: -0.49525 factor:1 | -1 (0.00805) | -1 | -1 |
| G: -5312.42844 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.96845 HOMO: -6.60692 LUMO: -0.22313 factor:1 | 1 (-0.17432) | -1 | -1 |
| G: -5312.42844 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.77359 HOMO: -7.20013 LUMO: 0.55239 factor:1 | -1 (0.02054) | -1 | -1 |
| G: -5312.42844 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.96737 HOMO: -6.60420 LUMO: -0.28028 factor:1 | 1 (-0.17323) | -1 | -1 |
| G: -5312.42844 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.77528 HOMO: -6.69128 LUMO: -0.30477 factor:1 | -1 (0.01886) | -1 | -1 |
| G: -5312.42844 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.98138 HOMO: -6.65591 LUMO: -0.25579 factor:1 | 1 (-0.18724) | -1 | -1 |
| G: -5312.42844 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.81403 HOMO: -6.69128 LUMO: 1.70888 factor:1 | 1 (-0.01989) | -1 | -1 |
| G: -5312.42844 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.43704 HOMO: -6.50080 LUMO: 1.87759 factor:1 | -1 (0.35710) | -1 | -1 |
| G: -5312.42844 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.65620 HOMO: -6.85727 LUMO: 1.99187 factor:1 | -1 (0.13793) | -1 | -1 |
| G: -5312.42844 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.51533 HOMO: -6.58788 LUMO: 1.79051 factor:1 | -1 (0.27881) | -1 | -1 |
| G: -5312.42844 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.85691 HOMO: -6.64230 LUMO: 2.16058 factor:1 | 1 (-0.06278) | -1 | -1 |
| G: -5312.42844 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.58203 HOMO: -6.58788 LUMO: 2.10616 factor:1 | -1 (0.21211) | -1 | -1 |
| G: -5312.42844 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.54646 HOMO: -7.01782 LUMO: 2.13609 factor:1 | -1 (0.24768) | -1 | -1 |
| G: -5312.42844 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.38580 HOMO: -6.31304 LUMO: 2.31841 factor:1 | -1 (0.40833) | -1 | -1 |
| G: -5312.42844 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.73158 HOMO: -6.94979 LUMO: 2.07895 factor:1 | -1 (0.06256) | -1 | -1 |
| G: -5312.42844 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.91675 HOMO: -6.88992 LUMO: 2.28031 factor:1 | 1 (-0.12261) | -1 | -1 |
| G: -5312.42844 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.91068 HOMO: -6.66407 LUMO: 2.07623 factor:1 | 1 (-0.11655) | -1 | -1 |
| G: -5312.42844 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.89278 HOMO: -6.52529 LUMO: 1.70071 factor:1 | 1 (-0.09864) | -1 | -1 |
| G: -5312.42844 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.01104 HOMO: -6.58788 LUMO: 1.57282 factor:1 | 1 (-0.21690) | -1 | -1 |
| G: -5312.42844 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.03980 HOMO: -6.55250 LUMO: 1.95378 factor:1 | 1 (-0.24566) | -1 | -1 |
| G: -5312.42844 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.92524 HOMO: -6.24773 LUMO: 1.77962 factor:1 | 1 (-0.13110) | -1 | -1 |
| G: -5312.42844 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.88745 HOMO: -6.31304 LUMO: 2.18507 factor:1 | 1 (-0.09331) | -1 | -1 |
| G: -5312.42844 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.84663 HOMO: -6.18243 LUMO: 2.01636 factor:1 | 1 (-0.05249) | -1 | -1 |
| G: -5312.42844 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.82842 HOMO: -6.99877 LUMO: 2.14970 factor:1 | 1 (-0.03429) | -1 | -1 |
| G: -5312.42844 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.72116 HOMO: -6.72665 LUMO: 2.07079 factor:1 | -1 (0.07298) | -1 | -1 |
| G: -5312.42844 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.69435 HOMO: -6.36202 LUMO: 2.17419 factor:1 | -1 (0.09978) | -1 | -1 |
| G: -5312.42844 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.71814 HOMO: -6.78652 LUMO: 2.05718 factor:1 | -1 (0.07600) | -1 | -1 |
| G: -5312.42844 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.92380 HOMO: -6.87360 LUMO: 2.34290 factor:1 | 1 (-0.12966) | -1 | -1 |
| G: -5312.42844 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.67005 HOMO: -6.62053 LUMO: 1.89391 factor:1 | 1 (-0.87591) | -1 | -1 |
| G: -5312.42844 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.79258 HOMO: -6.58788 LUMO: 1.83133 factor:1 | 1 (-0.99844) | -1 | -1 |
| G: -5312.42844 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.86420 HOMO: -7.08584 LUMO: 1.91568 factor:1 | 1 (-1.07006) | 1 | 1 |
| G: -5312.42844 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.47829 HOMO: -6.56883 LUMO: 1.81228 factor:1 | 1 (-0.68415) | -1 | -1 |
| G: -5312.42844 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.43505 HOMO: -6.66135 LUMO: 1.92384 factor:1 | 1 (-0.64091) | -1 | -1 |
| G: -5312.42844 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.44961 HOMO: -6.64502 LUMO: 2.15786 factor:1 | 1 (-0.65547) | -1 | -1 |
| G: -5312.42844 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.43265 HOMO: -6.71305 LUMO: 1.91840 factor:1 | 1 (-0.63852) | -1 | -1 |
| G: -5312.42844 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.28158 HOMO: -6.44094 LUMO: 1.74425 factor:1 | 1 (-0.48744) | -1 | -1 |
| G: -5312.42844 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.62134 HOMO: -6.51985 LUMO: 1.84221 factor:1 | 1 (-0.82720) | -1 | -1 |
| G: -5312.42844 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.47763 HOMO: -6.63414 LUMO: -0.24762 factor:1 | 1 (-0.68350) | -1 | -1 |
| G: -5312.42844 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.59516 HOMO: -6.60420 LUMO: -0.22585 factor:1 | 1 (-0.80102) | -1 | -1 |
| G: -5312.42844 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11578.21272 HOMO: -7.19741 LUMO: 0.58232 factor:1 | 1 (-1.41858) | -1 | -1 |
| G: -5312.42844 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11578.00401 HOMO: -6.77019 LUMO: -0.56872 factor:1 | 1 (-1.20987) | -1 | -1 |
| G: -5312.42844 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11578.02303 HOMO: -7.46136 LUMO: 0.28844 factor:1 | 1 (-1.22889) | -1 | -1 |
| G: -5312.42844 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11578.83529 HOMO: -6.60420 LUMO: -0.54151 factor:1 | 1 (-2.04115) | -1 | -1 |
| G: -5312.42844 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11578.98079 HOMO: -6.53890 LUMO: -0.46531 factor:1 | 1 (-2.18665) | -1 | -1 |
| G: -5312.42844 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.97506 HOMO: -6.81645 LUMO: -0.57144 factor:1 | 1 (-1.18092) | -1 | -1 |
| G: -5312.42844 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11578.15620 HOMO: -7.48041 LUMO: 0.28572 factor:1 | 1 (-1.36207) | -1 | -1 |
| G: -5312.42844 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.79141 HOMO: -6.75659 LUMO: -0.45715 factor:1 | 1 (-0.99727) | -1 | -1 |
| G: -5312.42844 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11578.04156 HOMO: -6.66135 LUMO: -0.41906 factor:1 | 1 (-1.24742) | -1 | -1 |
| G: -5312.42844 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.78665 HOMO: -6.55794 LUMO: -0.27483 factor:1 | 1 (-0.99251) | -1 | -1 |
| G: -5312.42844 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.80286 HOMO: -7.07496 LUMO: -0.63403 factor:1 | 1 (-1.00873) | -1 | -1 |
| G: -5312.42844 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.73818 HOMO: -7.12394 LUMO: 0.53334 factor:1 | 1 (-0.94404) | -1 | -1 |
| G: -5312.42844 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.59813 HOMO: -6.53617 LUMO: -0.25579 factor:1 | 1 (-0.80399) | -1 | -1 |
| G: -5312.42844 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.75245 HOMO: -6.50896 LUMO: -0.25034 factor:1 | -1 (0.04169) | -1 | -1 |
| G: -5312.42844 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.96494 HOMO: -7.17564 LUMO: -0.68573 factor:1 | 1 (-0.17081) | -1 | -1 |
| G: -5312.42844 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.84187 HOMO: -6.53617 LUMO: -0.30749 factor:1 | 1 (-0.04773) | -1 | -1 |
| G: -5312.42844 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.90619 HOMO: -6.55522 LUMO: -0.30749 factor:1 | 1 (-0.11206) | -1 | -1 |
| G: -5312.42844 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.92399 HOMO: -7.05591 LUMO: -0.71022 factor:1 | 1 (-0.12985) | -1 | -1 |
| G: -5312.42844 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.91158 HOMO: -7.17564 LUMO: -0.69933 factor:1 | 1 (-0.11744) | -1 | -1 |
| G: -5312.42844 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.82829 HOMO: -6.78380 LUMO: -0.67756 factor:1 | 1 (-0.03415) | -1 | -1 |
| G: -5312.42844 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.77049 HOMO: -6.62325 LUMO: 2.02725 factor:1 | -1 (0.02365) | -1 | -1 |
| G: -5312.42844 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.73539 HOMO: -6.63414 LUMO: 1.91296 factor:1 | -1 (0.05875) | -1 | -1 |
| G: -5312.42844 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.56192 HOMO: -6.83278 LUMO: 1.65717 factor:1 | -1 (0.23222) | -1 | -1 |
| G: -5312.42844 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.92170 HOMO: -6.66407 LUMO: 1.95650 factor:1 | 1 (-0.12757) | -1 | -1 |
| G: -5312.42844 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.75297 HOMO: -6.61237 LUMO: 2.11432 factor:1 | -1 (0.04117) | -1 | -1 |
| G: -5312.42844 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.69699 HOMO: -6.62053 LUMO: 2.09256 factor:1 | -1 (0.09714) | -1 | -1 |
| G: -5312.42844 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.98160 HOMO: -6.78652 LUMO: 2.13609 factor:1 | 1 (-0.18746) | -1 | -1 |
| G: -5312.42844 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.72401 HOMO: -6.94707 LUMO: 1.81772 factor:1 | -1 (0.07012) | -1 | -1 |
| G: -5312.42844 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.75727 HOMO: -6.85183 LUMO: 2.12793 factor:1 | -1 (0.03687) | -1 | -1 |
| G: -5312.42844 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.85528 HOMO: -6.81101 LUMO: 1.83949 factor:1 | 1 (-0.06114) | -1 | -1 |
| G: -5312.42844 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.76763 HOMO: -6.98788 LUMO: 2.16058 factor:1 | -1 (0.02650) | -1 | -1 |
| G: -5312.42844 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.92845 HOMO: -6.62869 LUMO: 2.00820 factor:1 | 1 (-0.13432) | -1 | -1 |
| G: -5312.42844 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.62467 HOMO: -6.34025 LUMO: 2.25855 factor:1 | -1 (0.16947) | -1 | -1 |
| G: -5312.42844 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.77778 HOMO: -6.01372 LUMO: 2.01636 factor:1 | -1 (0.01635) | -1 | -1 |
| G: -5312.42844 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.50012 HOMO: -6.89264 LUMO: 2.27487 factor:1 | -1 (0.29402) | -1 | -1 |
| G: -5312.42844 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.82051 HOMO: -6.53073 LUMO: 2.20684 factor:1 | 1 (-0.02637) | -1 | -1 |
| G: -5312.42844 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.71103 HOMO: -6.83278 LUMO: 1.53744 factor:1 | -1 (0.08310) | -1 | -1 |
| G: -5312.42844 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.78891 HOMO: -6.41917 LUMO: 1.82316 factor:1 | -1 (0.00522) | -1 | -1 |
| G: -5312.42844 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.69014 HOMO: -6.56339 LUMO: 1.63813 factor:1 | -1 (0.10400) | -1 | -1 |
| G: -5312.42844 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.82894 HOMO: -6.88992 LUMO: 1.65173 factor:1 | 1 (-0.03480) | -1 | -1 |
| G: -5312.42844 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.67944 HOMO: -6.63141 LUMO: 1.92112 factor:1 | -1 (0.11470) | -1 | -1 |
| G: -5312.42844 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.68910 HOMO: -6.83822 LUMO: 1.88847 factor:1 | -1 (0.10504) | -1 | -1 |
| G: -5312.42844 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.54450 HOMO: -6.84638 LUMO: 1.90480 factor:1 | -1 (0.24964) | -1 | -1 |
| G: -5312.42844 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.59109 HOMO: -6.82462 LUMO: 1.70888 factor:1 | -1 (0.20305) | -1 | -1 |
| G: -5312.42844 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.88883 HOMO: -6.82734 LUMO: 2.12521 factor:1 | 1 (-0.09470) | -1 | -1 |
| G: -5312.42844 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.73686 HOMO: -6.94435 LUMO: 1.87214 factor:1 | -1 (0.05728) | -1 | -1 |
| G: -5312.42844 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.79438 HOMO: -6.98516 LUMO: 2.51433 factor:1 | 1 (-0.00024) | -1 | -1 |
| G: -5312.42844 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: 2.15514 factor:1 | -1 (0.00112) | -1 | -1 |
| G: -5312.42844 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11578.18801 HOMO: -6.93618 LUMO: 2.54426 factor:1 | 1 (-1.39388) | -1 | -1 |
| G: -5312.42844 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11578.97167 HOMO: -6.28583 LUMO: 2.53610 factor:1 | 1 (-2.17754) | -1 | -1 |
| G: -5312.42844 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.98662 HOMO: -6.56883 LUMO: 1.94834 factor:1 | 1 (-1.19248) | -1 | -1 |
| G: -5312.42844 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11578.13373 HOMO: -7.08584 LUMO: 1.99187 factor:1 | 1 (-1.33959) | 1 | 1 |
| G: -5312.42844 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11578.14733 HOMO: -6.19059 LUMO: 1.99732 factor:1 | 1 (-1.35320) | -1 | -1 |
| G: -5312.42844 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11578.00404 HOMO: -6.78108 LUMO: 2.03813 factor:1 | 1 (-1.20990) | -1 | -1 |
| G: -5312.42844 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.68978 HOMO: -6.82189 LUMO: 1.77418 factor:1 | -1 (0.10436) | -1 | -1 |
| G: -5312.42844 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.74864 HOMO: -6.45454 LUMO: 1.78779 factor:1 | -1 (0.04550) | -1 | -1 |
| G: -5312.42844 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.75269 HOMO: -6.84366 LUMO: 1.77690 factor:1 | -1 (0.04144) | -1 | -1 |
| G: -5312.42844 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.55775 HOMO: -6.74026 LUMO: 1.67622 factor:1 | -1 (0.23639) | -1 | -1 |
| G: -5312.42844 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.61917 HOMO: -6.76475 LUMO: 2.40277 factor:1 | -1 (0.17497) | -1 | -1 |
| G: -5312.42844 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.43552 HOMO: -6.65863 LUMO: 1.86670 factor:1 | -1 (0.35862) | -1 | -1 |
| G: -5312.42844 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.42877 HOMO: -6.50080 LUMO: 1.93201 factor:1 | -1 (0.36537) | -1 | -1 |
| G: -5312.42844 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.81506 HOMO: -6.34842 LUMO: 1.70888 factor:1 | 1 (-0.02093) | -1 | -1 |
| G: -5312.42844 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.65373 HOMO: -6.60692 LUMO: 2.20140 factor:1 | -1 (0.14041) | -1 | -1 |
| G: -5312.42844 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.64442 HOMO: -6.74026 LUMO: 2.14970 factor:1 | -1 (0.14972) | -1 | -1 |
| G: -5312.42844 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.74826 HOMO: -6.63686 LUMO: 2.17419 factor:1 | -1 (0.04588) | -1 | -1 |
| G: -5312.42844 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11578.46035 HOMO: -6.81917 LUMO: 2.10072 factor:1 | 1 (-1.66621) | -1 | -1 |
| G: -5312.42844 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.67075 HOMO: -6.92802 LUMO: 2.04358 factor:1 | 1 (-0.87661) | -1 | -1 |
| G: -5312.42844 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.71456 HOMO: -6.56067 LUMO: -0.47620 factor:1 | 1 (-0.92043) | -1 | -1 |
| G: -5312.42844 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.74607 HOMO: -6.56611 LUMO: -0.77008 factor:1 | 1 (-0.95194) | -1 | -1 |
| G: -5312.42844 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.74722 HOMO: -6.78380 LUMO: -0.64763 factor:1 | 1 (-0.95308) | -1 | -1 |
| G: -5312.42844 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.60368 HOMO: -6.51985 LUMO: -0.24490 factor:1 | 1 (-0.80954) | -1 | -1 |
| G: -5312.42844 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.80047 HOMO: -6.52529 LUMO: -0.27483 factor:1 | 1 (-1.00633) | -1 | -1 |
| G: -5312.08193 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.03352 HOMO: -7.10489 LUMO: -0.62586 factor:1 | 1 (-0.58589) | -1 | -1 |
| G: -5312.08193 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.84902 HOMO: -7.18108 LUMO: 0.48980 factor:1 | 1 (-0.40140) | -1 | -1 |
| G: -5312.08193 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.57944 HOMO: -7.14299 LUMO: -0.63947 factor:1 | 1 (-0.13181) | -1 | -1 |
| G: -5312.08193 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11578.44220 HOMO: -6.70761 LUMO: -0.54423 factor:1 | 1 (-1.99457) | -1 | -1 |
| G: -5312.08193 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11578.06807 HOMO: -7.32258 LUMO: -1.03675 factor:1 | 1 (-1.62044) | -1 | -1 |
| G: -5312.08193 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11579.01581 HOMO: -6.65046 LUMO: -0.41361 factor:1 | 1 (-2.56818) | -1 | -1 |
| G: -5312.08193 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11578.14426 HOMO: -6.76475 LUMO: -0.60137 factor:1 | 1 (-1.69663) | -1 | -1 |
| G: -5312.08193 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11578.29803 HOMO: -6.77836 LUMO: -0.54423 factor:1 | 1 (-1.85040) | -1 | -1 |
| G: -5312.08193 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.87095 HOMO: -7.52395 LUMO: 0.26395 factor:1 | 1 (-1.42332) | -1 | -1 |
| G: -5312.08193 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.91870 HOMO: -6.93890 LUMO: -0.72382 factor:1 | 1 (-1.47107) | -1 | -1 |
| G: -5312.08193 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.90734 HOMO: -6.72938 LUMO: -0.47348 factor:1 | 1 (-0.45971) | -1 | -1 |
| G: -5312.08193 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.31279 HOMO: -6.66951 LUMO: -0.40817 factor:1 | 1 (-0.86516) | -1 | -1 |
| G: -5312.08193 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.94470 HOMO: -6.60420 LUMO: -0.19320 factor:1 | 1 (-0.49707) | -1 | -1 |
| G: -5312.08193 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.26729 HOMO: -6.67495 LUMO: -0.27211 factor:1 | 1 (-0.81966) | -1 | -1 |
| G: -5312.08193 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.20982 HOMO: -7.23823 LUMO: -0.62858 factor:1 | 1 (-0.76219) | -1 | -1 |
| G: -5312.08193 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.44933 HOMO: -7.27088 LUMO: 0.53334 factor:1 | 1 (-1.00171) | -1 | -1 |
| G: -5312.08193 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.61638 HOMO: -7.20013 LUMO: 0.59049 factor:1 | 1 (-1.16876) | -1 | -1 |
| G: -5312.08193 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.80545 HOMO: -6.60148 LUMO: -0.20953 factor:1 | 1 (-1.35782) | -1 | -1 |
| G: -5312.08193 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.94529 HOMO: -6.69400 LUMO: -0.51974 factor:1 | 1 (-1.49766) | -1 | -1 |
| G: -5312.08193 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.65973 HOMO: -7.40422 LUMO: -0.98777 factor:1 | 1 (-1.21210) | -1 | -1 |
| G: -5312.08193 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.23591 HOMO: -6.88176 LUMO: -0.71022 factor:1 | 1 (-0.78829) | -1 | -1 |
| G: -5312.08193 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.16650 HOMO: -6.86271 LUMO: -0.59321 factor:1 | 1 (-0.71887) | -1 | -1 |
| G: -5312.08193 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.81999 HOMO: -6.73754 LUMO: -0.55239 factor:1 | 1 (-0.37236) | -1 | -1 |
| G: -5312.08193 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.19684 HOMO: -6.71033 LUMO: 1.57010 factor:1 | 1 (-0.74921) | -1 | -1 |
| G: -5312.08193 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.95011 HOMO: -6.69672 LUMO: 1.68711 factor:1 | 1 (-0.50249) | -1 | -1 |
| G: -5312.08193 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.75980 HOMO: -6.67495 LUMO: 2.03813 factor:1 | 1 (-0.31217) | -1 | -1 |
| G: -5312.08193 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.04078 HOMO: -6.54434 LUMO: 1.83677 factor:1 | 1 (-0.59315) | -1 | -1 |
| G: -5312.08193 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.98805 HOMO: -6.57155 LUMO: 1.77146 factor:1 | 1 (-0.54042) | -1 | -1 |
| G: -5312.08193 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11578.40693 HOMO: -6.76747 LUMO: 1.87759 factor:1 | 1 (-1.95930) | -1 | -1 |
| G: -5312.08193 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.71807 HOMO: -6.58243 LUMO: 1.61364 factor:1 | 1 (-1.27045) | -1 | -1 |
| G: -5312.08193 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.81658 HOMO: -6.61781 LUMO: 2.13881 factor:1 | 1 (-1.36895) | -1 | -1 |
| G: -5312.08193 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11578.02926 HOMO: -6.62597 LUMO: 2.00276 factor:1 | 1 (-1.58163) | -1 | -1 |
| G: -5312.08193 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11578.34372 HOMO: -7.01237 LUMO: 1.95922 factor:1 | 1 (-1.89609) | -1 | -1 |
| G: -5312.08193 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11578.21977 HOMO: -7.03959 LUMO: 2.16875 factor:1 | 1 (-1.77214) | -1 | -1 |
| G: -5312.08193 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11578.26497 HOMO: -6.83278 LUMO: 1.91296 factor:1 | 1 (-1.81734) | -1 | -1 |
| G: -5312.08193 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11578.14668 HOMO: -6.40012 LUMO: 1.95650 factor:1 | 1 (-1.69905) | -1 | -1 |
| G: -5312.08193 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.03763 HOMO: -6.50080 LUMO: 1.73337 factor:1 | 1 (-0.59000) | -1 | -1 |
| G: -5312.08193 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.87120 HOMO: -6.95795 LUMO: 2.28848 factor:1 | 1 (-0.42357) | -1 | -1 |
| G: -5312.08193 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.07972 HOMO: -6.63686 LUMO: 2.20140 factor:1 | 1 (-0.63209) | -1 | -1 |
| G: -5312.08193 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11578.43659 HOMO: -6.57427 LUMO: 1.87214 factor:1 | 1 (-1.98896) | -1 | -1 |
| G: -5312.08193 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.90921 HOMO: -6.38379 LUMO: 2.32113 factor:1 | 1 (-1.46158) | -1 | -1 |
| G: -5312.08193 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.80221 HOMO: -6.63958 LUMO: 2.04902 factor:1 | 1 (-1.35458) | -1 | -1 |
| G: -5312.08193 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.90619 HOMO: -6.70216 LUMO: 1.93201 factor:1 | 1 (-1.45856) | -1 | -1 |
| G: -5312.08193 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11578.00703 HOMO: -6.80557 LUMO: 2.23678 factor:1 | 1 (-1.55940) | -1 | -1 |
| G: -5312.08193 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.87946 HOMO: -6.72938 LUMO: 2.28304 factor:1 | 1 (-1.43184) | -1 | -1 |
| G: -5312.08193 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.13657 HOMO: -6.56067 LUMO: 1.66806 factor:1 | 1 (-0.68894) | -1 | -1 |
| G: -5312.08193 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.05120 HOMO: -6.95523 LUMO: 2.33474 factor:1 | 1 (-0.60358) | -1 | -1 |
| G: -5312.08193 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.94410 HOMO: -6.59876 LUMO: 2.30480 factor:1 | 1 (-0.49647) | -1 | -1 |
| G: -5312.08193 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.12138 HOMO: -6.87360 LUMO: 1.75786 factor:1 | 1 (-0.67375) | -1 | -1 |
| G: -5312.08193 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.04282 HOMO: -7.06408 LUMO: 1.99187 factor:1 | 1 (-0.59519) | 1 | 1 |
| G: -5312.08193 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.03874 HOMO: -6.95795 LUMO: 1.88847 factor:1 | 1 (-0.59111) | -1 | -1 |
| G: -5312.08193 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.05523 HOMO: -6.85455 LUMO: 1.63813 factor:1 | 1 (-0.60760) | -1 | -1 |
| G: -5312.08193 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.92949 HOMO: -7.09129 LUMO: 2.31569 factor:1 | 1 (-0.48186) | 1 | 1 |
| G: -5312.08193 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.12590 HOMO: -6.91441 LUMO: 1.68983 factor:1 | 1 (-0.67827) | -1 | -1 |
| G: -5312.08193 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.08603 HOMO: -6.89809 LUMO: 2.23678 factor:1 | 1 (-0.63841) | -1 | -1 |
| G: -5312.08193 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.07700 HOMO: -6.78652 LUMO: 1.98371 factor:1 | 1 (-0.62937) | -1 | -1 |
| G: -5312.08193 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.84032 HOMO: -6.94707 LUMO: 2.23678 factor:1 | 1 (-0.39269) | -1 | -1 |
| G: -5312.08193 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.02666 HOMO: -7.07224 LUMO: 2.13337 factor:1 | 1 (-0.57903) | 1 | 1 |
| G: -5312.08193 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.85101 HOMO: -6.94979 LUMO: 2.28031 factor:1 | 1 (-0.40338) | -1 | -1 |
| G: -5312.08193 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.06329 HOMO: -6.60965 LUMO: 2.20412 factor:1 | 1 (-0.61566) | -1 | -1 |
| G: -5312.08193 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11579.05184 HOMO: -6.87360 LUMO: 2.40277 factor:1 | 1 (-2.60421) | -1 | -1 |
| G: -5312.08193 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11578.24889 HOMO: -6.92802 LUMO: 1.89663 factor:1 | 1 (-1.80126) | -1 | -1 |
| G: -5312.08193 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11578.30391 HOMO: -6.88448 LUMO: 2.02725 factor:1 | 1 (-1.85628) | -1 | -1 |
| G: -5312.08193 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.91966 HOMO: -6.69128 LUMO: 1.55105 factor:1 | 1 (-0.47204) | -1 | -1 |
| G: -5312.08193 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.90990 HOMO: -6.54978 LUMO: 1.93201 factor:1 | 1 (-0.46227) | -1 | -1 |
| G: -5312.08193 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.92821 HOMO: -6.19331 LUMO: 1.46941 factor:1 | 1 (-0.48058) | -1 | -1 |
| G: -5312.08193 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.01300 HOMO: -6.55794 LUMO: 1.89663 factor:1 | 1 (-0.56537) | -1 | -1 |
| G: -5312.08193 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11578.36530 HOMO: -6.07630 LUMO: 1.94289 factor:1 | 1 (-1.91767) | -1 | -1 |
| G: -5312.08193 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.72863 HOMO: -7.46408 LUMO: 0.31565 factor:1 | 1 (-1.28100) | -1 | -1 |
| G: -5312.08193 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.93634 HOMO: -6.63958 LUMO: -0.61770 factor:1 | 1 (-1.48871) | -1 | -1 |
| G: -5312.08193 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.90281 HOMO: -6.81101 LUMO: -0.57960 factor:1 | 1 (-1.45518) | -1 | -1 |
| G: -5312.08193 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.89751 HOMO: -6.74298 LUMO: -0.57960 factor:1 | 1 (-1.44988) | -1 | -1 |
| G: -5312.08193 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.93692 HOMO: -6.63686 LUMO: -0.42994 factor:1 | 1 (-0.48929) | -1 | -1 |
| G: -5312.08193 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.06900 HOMO: -6.60965 LUMO: -0.41089 factor:1 | 1 (-0.62137) | -1 | -1 |
| G: -5312.08193 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.92396 HOMO: -6.60692 LUMO: -0.80274 factor:1 | 1 (-0.47634) | -1 | -1 |
| G: -5312.08193 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.15140 HOMO: -6.58788 LUMO: -0.78097 factor:1 | 1 (-0.70377) | -1 | -1 |
| G: -5312.08193 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.18797 HOMO: -6.67767 LUMO: -0.48436 factor:1 | 1 (-0.74034) | -1 | -1 |
| G: -5312.08193 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.46615 HOMO: -6.63141 LUMO: -0.40545 factor:1 | 1 (-1.01852) | -1 | -1 |
| G: -5312.08193 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.13589 HOMO: -6.62053 LUMO: -0.83811 factor:1 | 1 (-0.68826) | -1 | -1 |
| G: -5312.08193 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.33159 HOMO: -6.59604 LUMO: -0.35375 factor:1 | 1 (-0.88396) | -1 | -1 |
| G: -5312.08193 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.22342 HOMO: -6.34297 LUMO: -0.39729 factor:1 | 1 (-0.77580) | -1 | -1 |
| G: -5312.08193 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.13433 HOMO: -6.67223 LUMO: 1.97827 factor:1 | 1 (-0.68671) | -1 | -1 |
| G: -5312.08193 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.29834 HOMO: -6.40012 LUMO: 1.89935 factor:1 | 1 (-0.85071) | -1 | -1 |
| G: -5312.08193 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.22571 HOMO: -6.74842 LUMO: 1.97283 factor:1 | 1 (-0.77808) | -1 | -1 |
| G: -5312.08193 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.12233 HOMO: -6.76747 LUMO: 2.17147 factor:1 | 1 (-0.67471) | -1 | -1 |
| G: -5312.08193 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.17338 HOMO: -6.72121 LUMO: 1.55649 factor:1 | 1 (-0.72575) | -1 | -1 |
| G: -5312.08193 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.99752 HOMO: -6.97700 LUMO: 2.04085 factor:1 | 1 (-0.54989) | -1 | -1 |
| G: -5312.08193 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.02682 HOMO: -7.06680 LUMO: 2.04085 factor:1 | 1 (-0.57919) | 1 | 1 |
| G: -5312.08193 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.08987 HOMO: -7.09673 LUMO: 2.35106 factor:1 | 1 (-0.64224) | 1 | 1 |
| G: -5312.08193 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.17028 HOMO: -6.83006 LUMO: 2.14970 factor:1 | 1 (-0.72265) | -1 | -1 |
| G: -5312.08193 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.28193 HOMO: -6.72665 LUMO: 2.20140 factor:1 | 1 (-0.83430) | -1 | -1 |
| G: -5312.08193 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.68126 HOMO: -6.77291 LUMO: 2.34562 factor:1 | 1 (-1.23363) | -1 | -1 |
| G: -5312.08193 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.87073 HOMO: -6.73754 LUMO: 2.00276 factor:1 | 1 (-1.42310) | -1 | -1 |
| G: -5312.08193 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.64139 HOMO: -7.04231 LUMO: 1.92112 factor:1 | 1 (-1.19376) | -1 | -1 |
| G: -5312.08193 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.89272 HOMO: -6.83822 LUMO: 1.72248 factor:1 | 1 (-1.44509) | -1 | -1 |
| G: -5312.08193 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.62999 HOMO: -6.57971 LUMO: 2.16603 factor:1 | 1 (-1.18236) | -1 | -1 |
| G: -5312.08193 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.95459 HOMO: -6.80013 LUMO: 1.88575 factor:1 | 1 (-1.50697) | -1 | -1 |
| G: -5312.08193 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.05490 HOMO: -6.93618 LUMO: 2.18235 factor:1 | 1 (-0.60728) | -1 | -1 |
| G: -5312.08193 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.99806 HOMO: -6.54706 LUMO: 1.91024 factor:1 | 1 (-0.55043) | -1 | -1 |
| G: -5312.08193 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.06497 HOMO: -7.06952 LUMO: 2.18507 factor:1 | 1 (-0.61734) | 1 | 1 |
| G: -5312.08193 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.12217 HOMO: -7.05047 LUMO: 1.82044 factor:1 | 1 (-0.67454) | -1 | -1 |
| G: -5312.08193 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.08105 HOMO: -6.87632 LUMO: 1.92657 factor:1 | 1 (-0.63343) | -1 | -1 |
| G: -5312.08193 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.15738 HOMO: -6.58788 LUMO: 1.91568 factor:1 | 1 (-0.70975) | -1 | -1 |
| G: -5312.08193 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.20478 HOMO: -7.17292 LUMO: 1.90752 factor:1 | 1 (-0.75716) | 1 | 1 |
| G: -5312.08193 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.15923 HOMO: -6.93890 LUMO: 1.80684 factor:1 | 1 (-0.71160) | -1 | -1 |
| G: -5312.08193 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.50906 HOMO: -7.10761 LUMO: 2.20956 factor:1 | 1 (-1.06143) | 1 | 1 |
| G: -5312.08193 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.31507 HOMO: -6.85727 LUMO: 2.13609 factor:1 | 1 (-0.86744) | -1 | -1 |
| G: -5312.08193 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.22440 HOMO: -6.64502 LUMO: 1.38506 factor:1 | 1 (-0.77678) | -1 | -1 |
| G: -5312.08193 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.26255 HOMO: -6.87360 LUMO: 1.15648 factor:1 | 1 (-0.81493) | -1 | -1 |
| G: -5312.08193 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.25654 HOMO: -6.67223 LUMO: 2.07351 factor:1 | 1 (-0.80891) | -1 | -1 |
| G: -5312.08193 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.12729 HOMO: -6.29671 LUMO: 2.43270 factor:1 | 1 (-0.67966) | -1 | -1 |
| G: -5312.08193 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.22789 HOMO: -6.90897 LUMO: 2.28848 factor:1 | 1 (-0.78026) | -1 | -1 |
| G: -5312.08193 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.18367 HOMO: -7.04231 LUMO: 1.70071 factor:1 | 1 (-0.73604) | -1 | -1 |
| G: -5312.08193 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.06089 HOMO: -6.69944 LUMO: 1.94834 factor:1 | 1 (-0.61326) | -1 | -1 |
| G: -5312.08193 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.70915 HOMO: -6.56067 LUMO: 2.20956 factor:1 | 1 (-1.26152) | -1 | -1 |
| G: -5312.08193 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.97250 HOMO: -6.65046 LUMO: 2.06807 factor:1 | 1 (-1.52487) | -1 | -1 |
| G: -5312.08193 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.98733 HOMO: -7.08584 LUMO: 1.98915 factor:1 | 1 (-1.53970) | 1 | 1 |
| G: -5312.08193 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.89506 HOMO: -6.69400 LUMO: 2.09256 factor:1 | 1 (-1.44743) | -1 | -1 |
| G: -5312.08193 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11578.00728 HOMO: -6.62869 LUMO: 2.16331 factor:1 | 1 (-1.55965) | -1 | -1 |
| G: -5312.08193 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.81571 HOMO: -6.85183 LUMO: 2.16058 factor:1 | 1 (-1.36808) | -1 | -1 |
| G: -5312.08193 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.80836 HOMO: -6.54706 LUMO: 1.92384 factor:1 | 1 (-1.36073) | -1 | -1 |
| G: -5312.08193 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.17161 HOMO: -6.84366 LUMO: 2.48984 factor:1 | 1 (-0.72399) | -1 | -1 |
| G: -5312.08193 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.31047 HOMO: -6.77291 LUMO: 2.46263 factor:1 | 1 (-0.86285) | -1 | -1 |
| G: -5312.08193 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.22168 HOMO: -7.01782 LUMO: 2.31025 factor:1 | 1 (-0.77406) | -1 | -1 |
| G: -5312.08193 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.13526 HOMO: -6.94707 LUMO: 2.29664 factor:1 | 1 (-0.68763) | -1 | -1 |
| G: -5312.08193 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.58749 HOMO: -6.64230 LUMO: 1.97283 factor:1 | 1 (-1.13986) | -1 | -1 |
| G: -5312.08193 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.71002 HOMO: -6.47359 LUMO: 2.20412 factor:1 | 1 (-1.26239) | -1 | -1 |
| G: -5312.08193 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.74716 HOMO: -6.90625 LUMO: 1.92384 factor:1 | 1 (-1.29953) | -1 | -1 |
| G: -5312.08193 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.88082 HOMO: -7.17020 LUMO: 2.06807 factor:1 | 1 (-1.43320) | 1 | 1 |
| G: -5312.08193 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.70433 HOMO: -6.65046 LUMO: 2.20956 factor:1 | 1 (-1.25670) | -1 | -1 |
| G: -5312.08193 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.57698 HOMO: -7.07496 LUMO: 1.82861 factor:1 | 1 (-1.12935) | 1 | 1 |
| G: -5312.08193 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.69598 HOMO: -6.83006 LUMO: 2.14970 factor:1 | 1 (-1.24835) | -1 | -1 |
| G: -5312.08193 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.75065 HOMO: -6.92802 LUMO: 1.99187 factor:1 | 1 (-1.30302) | -1 | -1 |
| G: -5312.08193 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.51976 HOMO: -6.69672 LUMO: 2.36739 factor:1 | 1 (-1.07213) | -1 | -1 |
| G: -5312.08193 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.58476 HOMO: -7.13755 LUMO: 2.00276 factor:1 | 1 (-1.13714) | 1 | 1 |
| G: -5312.08193 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.88763 HOMO: -6.92530 LUMO: 2.25582 factor:1 | 1 (-1.44000) | -1 | -1 |
| G: -5312.08193 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.91780 HOMO: -6.77564 LUMO: 1.97827 factor:1 | 1 (-1.47018) | -1 | -1 |
| G: -5312.08193 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.67233 HOMO: -6.87904 LUMO: 1.60003 factor:1 | 1 (-1.22470) | -1 | -1 |
| G: -5312.08193 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.71426 HOMO: -6.62869 LUMO: 1.90480 factor:1 | 1 (-1.26664) | -1 | -1 |
| G: -5312.08193 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11578.38712 HOMO: -6.71033 LUMO: 1.54833 factor:1 | 1 (-1.93949) | -1 | -1 |
| G: -5312.08193 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11579.11660 HOMO: -6.74298 LUMO: 1.47486 factor:1 | 1 (-2.66897) | -1 | -1 |
| G: -5312.08193 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11578.42862 HOMO: -6.77019 LUMO: 1.90480 factor:1 | 1 (-1.98099) | -1 | -1 |
| G: -5312.08193 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.91500 HOMO: -6.70489 LUMO: 1.99459 factor:1 | 1 (-1.46737) | -1 | -1 |