乙二醇作为反应物的反应表19-2

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: -4242.91430 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10508.62851 HOMO: -6.91169 LUMO: -0.53879 factor:1 | 1 (-1.34851) | -1 | -1 |
| G: -4242.91430 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10508.58285 HOMO: -7.29809 LUMO: 2.83543 factor:1 | 1 (-1.30285) | 1 | -1 |
| G: -4242.91430 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10508.60402 HOMO: -6.86543 LUMO: -0.70205 factor:1 | 1 (-1.32402) | -1 | -1 |
| G: -4242.91430 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10508.72688 HOMO: -7.47769 LUMO: 0.31293 factor:1 | 1 (-1.44688) | -1 | -1 |
| G: -4242.91430 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10508.43450 HOMO: -6.63141 LUMO: -0.55511 factor:1 | 1 (-1.15450) | -1 | -1 |
| G: -4242.91430 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10508.88844 HOMO: -6.68856 LUMO: -0.30205 factor:1 | 1 (-1.60844) | -1 | -1 |
| G: -4242.91430 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10508.45373 HOMO: -7.22190 LUMO: 0.53334 factor:1 | 1 (-1.17374) | -1 | -1 |
| G: -4242.91430 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10508.23942 HOMO: -6.66407 LUMO: -0.27756 factor:1 | 1 (-0.95942) | -1 | -1 |
| G: -4242.91430 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10508.32530 HOMO: -7.15659 LUMO: -0.70205 factor:1 | 1 (-1.04530) | -1 | -1 |
| G: -4242.91430 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10508.18951 HOMO: -6.69400 LUMO: 1.67622 factor:1 | 1 (-0.90951) | -1 | -1 |
| G: -4242.91430 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10508.08682 HOMO: -6.60420 LUMO: 2.16058 factor:1 | 1 (-0.80682) | -1 | -1 |
| G: -4242.91430 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10508.54359 HOMO: -6.87087 LUMO: 1.88031 factor:1 | 1 (-1.26359) | -1 | -1 |
| G: -4242.91430 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10508.26943 HOMO: -6.60965 LUMO: -0.19864 factor:1 | 1 (-0.98943) | -1 | -1 |
| G: -4242.91430 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10508.33833 HOMO: -7.29265 LUMO: 0.52246 factor:1 | 1 (-1.05833) | -1 | -1 |
| G: -4242.91430 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10508.54756 HOMO: -6.86543 LUMO: -0.59593 factor:1 | 1 (-1.26756) | -1 | -1 |
| G: -4242.91430 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10508.68860 HOMO: -7.44504 LUMO: -1.01226 factor:1 | 1 (-1.40860) | -1 | -1 |
| G: -4242.91430 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10508.61349 HOMO: -6.92530 LUMO: -0.75103 factor:1 | 1 (-1.33349) | -1 | -1 |
| G: -4242.91430 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10508.54862 HOMO: -7.10489 LUMO: 2.20412 factor:1 | 1 (-1.26862) | 1 | 1 |
| G: -4242.91430 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10507.75554 HOMO: -6.58788 LUMO: 1.73881 factor:1 | 1 (-0.47555) | -1 | -1 |
| G: -4242.91430 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10507.73100 HOMO: -6.64502 LUMO: 1.70343 factor:1 | 1 (-0.45100) | -1 | -1 |
| G: -4242.91430 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10507.85582 HOMO: -6.73754 LUMO: 1.60819 factor:1 | 1 (-0.57582) | -1 | -1 |
| G: -4242.91430 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10507.87802 HOMO: -6.80829 LUMO: 2.45991 factor:1 | 1 (-0.59802) | -1 | -1 |
| G: -4242.91430 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10507.77481 HOMO: -6.91713 LUMO: 2.43814 factor:1 | 1 (-0.49481) | -1 | -1 |
| G: -4242.91430 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10507.58098 HOMO: -6.60692 LUMO: 1.93745 factor:1 | 1 (-0.30099) | -1 | -1 |
| G: -4242.91430 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10507.53960 HOMO: -6.26134 LUMO: 1.46125 factor:1 | 1 (-0.25960) | -1 | -1 |
| G: -4242.91430 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10507.52504 HOMO: -7.54028 LUMO: 0.25851 factor:1 | 1 (-0.24504) | -1 | -1 |
| G: -4242.91430 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10507.78553 HOMO: -6.97700 LUMO: -0.73471 factor:1 | 1 (-0.50553) | -1 | -1 |
| G: -4242.91430 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10507.75285 HOMO: -6.92258 LUMO: -0.70205 factor:1 | 1 (-0.47285) | -1 | -1 |
| G: -4242.91430 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10507.58618 HOMO: -6.83550 LUMO: -0.56872 factor:1 | 1 (-0.30618) | -1 | -1 |
| G: -4242.91430 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10507.96420 HOMO: -6.72121 LUMO: 1.89663 factor:1 | 1 (-0.68420) | -1 | -1 |
| G: -4242.91430 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10507.73593 HOMO: -6.73482 LUMO: 1.89935 factor:1 | 1 (-0.45593) | -1 | -1 |
| G: -4242.91430 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10507.60245 HOMO: -6.61781 LUMO: 1.86670 factor:1 | 1 (-0.32245) | -1 | -1 |
| G: -4242.91430 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10507.45306 HOMO: -7.01782 LUMO: 2.26399 factor:1 | 1 (-0.17306) | -1 | -1 |
| G: -4242.91430 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10507.86115 HOMO: -7.23551 LUMO: 2.09800 factor:1 | 1 (-0.58115) | 1 | 1 |
| G: -4242.91430 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10507.56302 HOMO: -7.13483 LUMO: 2.17963 factor:1 | 1 (-0.28303) | 1 | 1 |
| G: -4242.91430 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10507.63198 HOMO: -6.22869 LUMO: 2.01092 factor:1 | 1 (-0.35198) | -1 | -1 |
| G: -4242.91430 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10507.52991 HOMO: -6.80285 LUMO: 2.14970 factor:1 | 1 (-0.24991) | -1 | -1 |
| G: -4242.91430 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10507.53015 HOMO: -7.21102 LUMO: 2.33746 factor:1 | 1 (-0.25015) | 1 | 1 |
| G: -4242.91430 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10507.37701 HOMO: -6.39740 LUMO: 2.59597 factor:1 | 1 (-0.09701) | -1 | -1 |
| G: -4242.91430 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10507.72648 HOMO: -7.07768 LUMO: 2.48168 factor:1 | 1 (-0.44648) | 1 | 1 |
| G: -4242.91430 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10507.58471 HOMO: -7.11306 LUMO: 0.90614 factor:1 | 1 (-0.30471) | -1 | -1 |
| G: -4242.91430 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10507.73843 HOMO: -6.61781 LUMO: -2.46263 factor:1 | 1 (-0.45843) | -1 | -1 |
| G: -4242.91430 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10508.51156 HOMO: -6.96611 LUMO: 0.90614 factor:1 | 1 (-1.23156) | -1 | -1 |
| G: -4242.91430 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10508.62699 HOMO: -6.86271 LUMO: -1.14832 factor:1 | 1 (-1.34699) | -1 | -1 |
| G: -4242.91430 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10508.71194 HOMO: -6.72665 LUMO: 0.96873 factor:1 | 1 (-1.43194) | -1 | -1 |
| G: -4242.91430 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10508.31621 HOMO: -7.14571 LUMO: 1.05036 factor:1 | 1 (-1.03621) | -1 | -1 |
| G: -4242.91430 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10508.23283 HOMO: -7.14299 LUMO: 0.98777 factor:1 | 1 (-0.95283) | -1 | -1 |
| G: -4242.91430 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10508.14241 HOMO: -6.99333 LUMO: 1.05852 factor:1 | 1 (-0.86241) | -1 | -1 |
| G: -4242.91430 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10508.46584 HOMO: -6.78924 LUMO: -1.49935 factor:1 | 1 (-1.18584) | -1 | -1 |
| G: -4242.91430 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10508.33253 HOMO: -7.13755 LUMO: 0.94151 factor:1 | 1 (-1.05254) | -1 | -1 |
| G: -4242.91430 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10507.84782 HOMO: -6.72938 LUMO: -0.35375 factor:1 | 1 (-0.56782) | -1 | -1 |
| G: -4242.91430 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10507.77217 HOMO: -6.99061 LUMO: 0.82450 factor:1 | 1 (-0.49217) | -1 | -1 |
| G: -4242.91430 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10507.63620 HOMO: -6.75114 LUMO: -0.68028 factor:1 | 1 (-0.35620) | -1 | -1 |
| G: -4242.91430 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10507.46087 HOMO: -6.40556 LUMO: -0.42722 factor:1 | 1 (-0.18087) | -1 | -1 |
| G: -4242.91430 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10507.87827 HOMO: -7.18653 LUMO: 0.42178 factor:1 | 1 (-0.59827) | -1 | -1 |
| G: -4242.91430 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10507.88725 HOMO: -6.63958 LUMO: -0.71294 factor:1 | 1 (-0.60725) | -1 | -1 |
| G: -4242.91430 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10507.89723 HOMO: -6.63958 LUMO: -0.71022 factor:1 | 1 (-0.61724) | -1 | -1 |
| G: -4242.91430 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10507.90240 HOMO: -6.69672 LUMO: -0.72654 factor:1 | 1 (-0.62241) | -1 | -1 |
| G: -4242.91430 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10507.72651 HOMO: -6.56883 LUMO: -0.80274 factor:1 | 1 (-0.44651) | -1 | -1 |
| G: -4242.91430 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10507.82480 HOMO: -6.68584 LUMO: -0.56872 factor:1 | 1 (-0.54480) | -1 | -1 |
| G: -4242.91430 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10507.85519 HOMO: -6.59060 LUMO: -0.35647 factor:1 | 1 (-0.57519) | -1 | -1 |
| G: -4242.91430 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10507.89391 HOMO: -6.72121 LUMO: -0.71838 factor:1 | 1 (-0.61392) | -1 | -1 |
| G: -4242.91430 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10507.93691 HOMO: -6.57971 LUMO: -0.61498 factor:1 | 1 (-0.65691) | -1 | -1 |
| G: -4242.91430 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10507.57492 HOMO: -7.07496 LUMO: 0.50613 factor:1 | 1 (-0.29492) | -1 | -1 |
| G: -4242.91430 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10507.52599 HOMO: -7.14027 LUMO: 0.43266 factor:1 | 1 (-0.24599) | -1 | -1 |
| G: -4242.91430 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10507.61954 HOMO: -6.43277 LUMO: -0.44082 factor:1 | 1 (-0.33954) | -1 | -1 |
| G: -4242.91430 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10507.80727 HOMO: -6.79468 LUMO: 0.07619 factor:1 | 1 (-0.52728) | -1 | -1 |
| G: -4242.91430 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10507.57470 HOMO: -6.81917 LUMO: -2.57148 factor:1 | 1 (-0.29470) | -1 | -1 |
| G: -4242.91430 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10507.60422 HOMO: -6.71849 LUMO: 1.30615 factor:1 | 1 (-0.32422) | -1 | -1 |
| G: -4242.91430 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10507.69715 HOMO: -6.85455 LUMO: -0.63675 factor:1 | 1 (-0.41715) | -1 | -1 |
| G: -4242.91430 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10507.47124 HOMO: -6.73210 LUMO: -1.03131 factor:1 | 1 (-0.19124) | -1 | -1 |
| G: -4242.91430 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10507.62014 HOMO: -6.83550 LUMO: -0.58777 factor:1 | 1 (-0.34014) | -1 | -1 |
| G: -4242.91430 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10507.66645 HOMO: -6.53073 LUMO: -0.74287 factor:1 | 1 (-0.38646) | -1 | -1 |
| G: -4242.91430 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10507.85797 HOMO: -7.18381 LUMO: -0.92791 factor:1 | 1 (-0.57797) | -1 | -1 |
| G: -4242.91430 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10507.93204 HOMO: -6.49264 LUMO: -0.44627 factor:1 | 1 (-0.65204) | -1 | -1 |
| G: -4242.91430 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10507.98970 HOMO: -7.32803 LUMO: 0.41361 factor:1 | 1 (-0.70970) | -1 | -1 |
| G: -4242.91430 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10507.58765 HOMO: -6.53073 LUMO: -0.52790 factor:1 | 1 (-0.30765) | -1 | -1 |
| G: -4242.91430 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10508.47325 HOMO: -6.54978 LUMO: -0.53062 factor:1 | 1 (-1.19325) | -1 | -1 |
| G: -4242.91430 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10508.65412 HOMO: -6.56611 LUMO: -0.37824 factor:1 | 1 (-1.37412) | -1 | -1 |
| G: -4242.91430 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10508.69317 HOMO: -6.57155 LUMO: -0.64219 factor:1 | 1 (-1.41317) | -1 | -1 |
| G: -4242.91430 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10508.44680 HOMO: -7.08040 LUMO: 0.45715 factor:1 | 1 (-1.16680) | -1 | -1 |
| G: -4242.91430 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10507.80458 HOMO: -6.66679 LUMO: -0.75376 factor:1 | 1 (-0.52458) | -1 | -1 |
| G: -4242.91430 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10507.90972 HOMO: -6.83550 LUMO: -0.99322 factor:1 | 1 (-0.62973) | -1 | -1 |
| G: -4242.91430 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10509.30317 HOMO: -6.53345 LUMO: -0.29660 factor:1 | 1 (-2.02317) | -1 | -1 |
| G: -4242.91430 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10508.51365 HOMO: -6.65046 LUMO: 2.40549 factor:1 | 1 (-1.23366) | -1 | -1 |
| G: -4242.91430 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10508.56209 HOMO: -6.98788 LUMO: 2.01092 factor:1 | 1 (-1.28209) | -1 | -1 |
| G: -4242.91430 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10508.59529 HOMO: -6.61781 LUMO: 1.92384 factor:1 | 1 (-1.31529) | -1 | -1 |
| G: -4242.91430 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10508.44677 HOMO: -6.61237 LUMO: 2.06807 factor:1 | 1 (-1.16677) | -1 | -1 |
| G: -4242.91430 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10508.64465 HOMO: -6.59060 LUMO: 1.95106 factor:1 | 1 (-1.36465) | -1 | -1 |
| G: -4242.91430 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10507.77500 HOMO: -6.48175 LUMO: 1.72248 factor:1 | 1 (-0.49500) | -1 | -1 |
| G: -4242.91430 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10507.73573 HOMO: -6.84911 LUMO: 2.03541 factor:1 | 1 (-0.45574) | -1 | -1 |
| G: -4242.91430 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10507.61998 HOMO: -6.50624 LUMO: 2.17147 factor:1 | 1 (-0.33998) | -1 | -1 |
| G: -4242.91430 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10507.55472 HOMO: -6.68312 LUMO: 2.08439 factor:1 | 1 (-0.27473) | -1 | -1 |
| G: -4242.91430 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10507.29423 HOMO: -6.96067 LUMO: 1.98099 factor:1 | 1 (-0.01423) | -1 | -1 |
| G: -4242.91430 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10507.59783 HOMO: -6.93618 LUMO: 1.85854 factor:1 | 1 (-0.31783) | -1 | -1 |
| G: -4242.91430 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10508.63624 HOMO: -6.71305 LUMO: -0.61226 factor:1 | 1 (-1.35624) | -1 | -1 |
| G: -4242.91430 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10508.41216 HOMO: -7.06408 LUMO: 0.80001 factor:1 | 1 (-1.13216) | -1 | -1 |
| G: -4242.91430 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10508.47178 HOMO: -6.52257 LUMO: 0.99049 factor:1 | 1 (-1.19178) | -1 | -1 |
| G: -4242.91430 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10508.72032 HOMO: -6.84638 LUMO: 1.10750 factor:1 | 1 (-1.44033) | -1 | -1 |
| G: -4242.91430 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10508.57831 HOMO: -6.85455 LUMO: 0.84900 factor:1 | 1 (-1.29831) | -1 | -1 |
| G: -4242.91430 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10508.27207 HOMO: -6.60148 LUMO: -0.78369 factor:1 | 1 (-0.99207) | -1 | -1 |
| G: -4242.91430 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10508.29672 HOMO: -6.86543 LUMO: -0.93063 factor:1 | 1 (-1.01673) | -1 | -1 |
| G: -4242.91430 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10508.63368 HOMO: -6.70489 LUMO: -0.72382 factor:1 | 1 (-1.35368) | -1 | -1 |
| G: -4242.91430 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10508.44130 HOMO: -6.59060 LUMO: 0.31293 factor:1 | 1 (-1.16130) | -1 | -1 |
| G: -4242.91430 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10508.45341 HOMO: -6.52257 LUMO: -0.48708 factor:1 | 1 (-1.17341) | -1 | -1 |
| G: -4242.91430 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10507.69971 HOMO: -6.54706 LUMO: -0.48164 factor:1 | 1 (-0.41971) | -1 | -1 |
| G: -4242.91430 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10507.44403 HOMO: -7.32803 LUMO: 0.08436 factor:1 | 1 (-0.16403) | -1 | -1 |
| G: -4242.91430 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10507.47935 HOMO: -6.77291 LUMO: -0.66940 factor:1 | 1 (-0.19935) | -1 | -1 |
| G: -4242.91430 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10507.59595 HOMO: -6.68312 LUMO: -0.53062 factor:1 | 1 (-0.31595) | -1 | -1 |
| G: -4242.91430 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10507.52765 HOMO: -7.07768 LUMO: 0.45987 factor:1 | 1 (-0.24765) | -1 | -1 |
| G: -4242.91430 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10507.59206 HOMO: -6.50352 LUMO: -0.63675 factor:1 | 1 (-0.31206) | -1 | -1 |
| G: -4242.91430 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10507.45151 HOMO: -6.48992 LUMO: -0.60681 factor:1 | 1 (-0.17151) | -1 | -1 |
| G: -4242.91430 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10507.25679 HOMO: -6.65318 LUMO: -0.72382 factor:1 | -1 (0.02321) | -1 | -1 |
| G: -4242.91430 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10507.65731 HOMO: -6.54706 LUMO: 0.24218 factor:1 | 1 (-0.37731) | -1 | -1 |
| G: -4242.91430 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10507.47557 HOMO: -6.63958 LUMO: 0.57416 factor:1 | 1 (-0.19557) | -1 | -1 |
| G: -4242.91430 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10507.58610 HOMO: -6.37563 LUMO: -0.48164 factor:1 | 1 (-0.30610) | -1 | -1 |
| G: -4242.91430 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10507.60732 HOMO: -6.64774 LUMO: -0.71838 factor:1 | 1 (-0.32733) | -1 | -1 |
| G: -4242.91430 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10507.75682 HOMO: -7.17020 LUMO: 0.45987 factor:1 | 1 (-0.47683) | -1 | -1 |
| G: -4242.91430 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10507.47519 HOMO: -6.86543 LUMO: -1.05036 factor:1 | 1 (-0.19519) | -1 | -1 |
| G: -4242.91430 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10507.47908 HOMO: -6.77019 LUMO: -1.03131 factor:1 | 1 (-0.19908) | -1 | -1 |
| G: -4242.91430 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10507.17578 HOMO: -6.80285 LUMO: 1.05852 factor:1 | -1 (0.10422) | -1 | -1 |
| G: -4242.91430 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10507.81204 HOMO: -6.76475 LUMO: 1.01771 factor:1 | 1 (-0.53204) | -1 | -1 |
| G: -4242.91430 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10507.55818 HOMO: -6.92530 LUMO: 1.37417 factor:1 | 1 (-0.27818) | -1 | -1 |
| G: -4242.91430 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10507.82420 HOMO: -6.98244 LUMO: 1.25989 factor:1 | 1 (-0.54420) | -1 | -1 |
| G: -4242.91430 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10507.65954 HOMO: -6.74842 LUMO: 0.89798 factor:1 | 1 (-0.37954) | -1 | -1 |
| G: -4242.91430 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10507.23496 HOMO: -6.77019 LUMO: -1.17009 factor:1 | -1 (0.04503) | -1 | -1 |
| G: -4242.91430 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10507.42411 HOMO: -6.78652 LUMO: 1.35785 factor:1 | 1 (-0.14411) | -1 | -1 |
| G: -4242.91430 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10507.35717 HOMO: -6.82734 LUMO: -0.68301 factor:1 | 1 (-0.07717) | -1 | -1 |
| G: -4242.91430 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10507.21834 HOMO: -6.48175 LUMO: -2.19052 factor:1 | -1 (0.06166) | -1 | -1 |
| G: -4242.91430 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10507.57649 HOMO: -6.65863 LUMO: -0.77008 factor:1 | 1 (-0.29650) | -1 | -1 |
| G: -4242.91430 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10508.48530 HOMO: -6.44094 LUMO: -2.20956 factor:1 | 1 (-1.20530) | -1 | -1 |
| G: -4242.91430 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10508.29566 HOMO: -6.59876 LUMO: -0.57688 factor:1 | 1 (-1.01566) | -1 | -1 |
| G: -4242.91430 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10508.40783 HOMO: -6.78380 LUMO: -0.77008 factor:1 | 1 (-1.12783) | -1 | -1 |
| G: -4242.91430 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10508.43286 HOMO: -7.30354 LUMO: 0.25034 factor:1 | 1 (-1.15286) | -1 | -1 |
| G: -4242.91430 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10508.55385 HOMO: -6.59332 LUMO: -0.53334 factor:1 | 1 (-1.27385) | -1 | -1 |
| G: -4242.91430 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10508.61610 HOMO: -6.64230 LUMO: -0.55783 factor:1 | 1 (-1.33611) | -1 | -1 |
| G: -4242.91430 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10508.26380 HOMO: -7.26544 LUMO: 0.20409 factor:1 | 1 (-0.98380) | -1 | -1 |
| G: -4242.91430 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10508.30872 HOMO: -6.61237 LUMO: -0.65307 factor:1 | 1 (-1.02873) | -1 | -1 |
| G: -4242.91430 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10508.20472 HOMO: -6.72393 LUMO: -0.65307 factor:1 | 1 (-0.92472) | -1 | -1 |
| G: -4242.91430 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10508.61009 HOMO: -6.29671 LUMO: -0.39729 factor:1 | 1 (-1.33009) | -1 | -1 |
| G: -4242.91430 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10508.53550 HOMO: -6.75387 LUMO: -0.53334 factor:1 | 1 (-1.25551) | -1 | -1 |
| G: -4242.91430 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10507.62654 HOMO: -6.53073 LUMO: -0.31293 factor:1 | 1 (-0.34654) | -1 | -1 |
| G: -4242.91430 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10507.86619 HOMO: -6.42189 LUMO: -0.59049 factor:1 | 1 (-0.58619) | -1 | -1 |
| G: -4242.91430 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10507.64036 HOMO: -6.41100 LUMO: -0.29933 factor:1 | 1 (-0.36036) | -1 | -1 |
| G: -4242.91430 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10507.43567 HOMO: -6.57427 LUMO: -0.53879 factor:1 | 1 (-0.15568) | -1 | -1 |
| G: -4242.91430 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10507.49731 HOMO: -7.43143 LUMO: 0.33470 factor:1 | 1 (-0.21731) | -1 | -1 |
| G: -4242.91430 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10507.73677 HOMO: -6.56067 LUMO: -0.50885 factor:1 | 1 (-0.45677) | -1 | -1 |
| G: -4242.91430 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10507.91288 HOMO: -6.65863 LUMO: -0.76464 factor:1 | 1 (-0.63288) | -1 | -1 |
| G: -4242.91430 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10507.90632 HOMO: -6.32665 LUMO: -0.41906 factor:1 | 1 (-0.62632) | -1 | -1 |
| G: -4242.91430 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10507.97672 HOMO: -6.57699 LUMO: 1.63813 factor:1 | 1 (-0.69672) | -1 | -1 |
| G: -4242.91430 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10507.77783 HOMO: -6.53073 LUMO: 1.71704 factor:1 | 1 (-0.49783) | -1 | -1 |
| G: -4242.91430 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10507.80986 HOMO: -6.86271 LUMO: 2.07351 factor:1 | 1 (-0.52986) | -1 | -1 |
| G: -4242.91430 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10507.84341 HOMO: -6.63686 LUMO: 1.78235 factor:1 | 1 (-0.56341) | -1 | -1 |
| G: -4242.91430 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10507.78123 HOMO: -6.60965 LUMO: 1.94289 factor:1 | 1 (-0.50123) | -1 | -1 |
| G: -4242.91430 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10507.86281 HOMO: -6.55250 LUMO: 1.89119 factor:1 | 1 (-0.58281) | -1 | -1 |
| G: -4242.91430 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10507.76319 HOMO: -6.50624 LUMO: 1.85582 factor:1 | 1 (-0.48319) | -1 | -1 |
| G: -4242.91430 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10508.26442 HOMO: -6.06814 LUMO: 1.94561 factor:1 | 1 (-0.98443) | -1 | -1 |
| G: -4242.91430 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10507.93675 HOMO: -6.58788 LUMO: 2.01908 factor:1 | 1 (-0.65675) | -1 | -1 |
| G: -4681.25164 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10944.46792 HOMO: -6.74026 LUMO: 0.31293 factor:1 | -1 (1.14941) | -1 | -1 |
| G: -4681.25164 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10944.39002 HOMO: -6.54434 LUMO: -0.42994 factor:1 | -1 (1.22732) | -1 | -1 |
| G: -4681.25164 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10944.30204 HOMO: -6.94707 LUMO: 0.42994 factor:1 | -1 (1.31529) | -1 | -1 |
| G: -4681.25164 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10944.21396 HOMO: -6.98516 LUMO: 0.41361 factor:1 | -1 (1.40337) | -1 | -1 |
| G: -4681.25164 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10944.09681 HOMO: -6.31304 LUMO: -0.54967 factor:1 | -1 (1.52052) | -1 | -1 |
| G: -4681.25164 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10944.25031 HOMO: -6.48447 LUMO: -0.40817 factor:1 | -1 (1.36702) | -1 | -1 |
| G: -4681.25164 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10943.99153 HOMO: -6.49264 LUMO: 0.29116 factor:1 | -1 (1.62580) | -1 | -1 |
| G: -4681.25164 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10944.24204 HOMO: -6.48719 LUMO: -0.11973 factor:1 | -1 (1.37529) | -1 | -1 |
| G: -4681.25164 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10944.26555 HOMO: -7.16204 LUMO: 0.44082 factor:1 | -1 (1.35178) | -1 | -1 |
| G: -4681.25164 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10944.33690 HOMO: -6.74842 LUMO: -0.37552 factor:1 | -1 (1.28043) | -1 | -1 |
| G: -4681.25164 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10944.28452 HOMO: -6.44638 LUMO: -0.45171 factor:1 | -1 (1.33281) | -1 | -1 |
| G: -4681.25164 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10944.39176 HOMO: -7.07496 LUMO: 0.50341 factor:1 | -1 (1.22557) | -1 | -1 |
| G: -4681.25164 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10944.13257 HOMO: -6.79468 LUMO: 0.11429 factor:1 | -1 (1.48476) | -1 | -1 |
| G: -4681.25164 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10947.02664 HOMO: -6.63958 LUMO: -0.67484 factor:1 | 1 (-1.40930) | -1 | -1 |
| G: -4681.25164 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10944.68387 HOMO: -7.08584 LUMO: 0.46259 factor:1 | -1 (0.93346) | -1 | -1 |
| G: -4681.25164 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10946.71790 HOMO: -6.80285 LUMO: -0.73199 factor:1 | 1 (-1.10056) | -1 | -1 |
| G: -4681.25164 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10946.52725 HOMO: -6.44366 LUMO: -0.45443 factor:1 | 1 (-0.90992) | -1 | -1 |
| G: -4681.25164 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10946.30929 HOMO: -6.75931 LUMO: 0.25851 factor:1 | 1 (-0.69196) | -1 | -1 |
| G: -4681.25164 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10945.43629 HOMO: -6.64502 LUMO: 1.79323 factor:1 | -1 (0.18104) | -1 | -1 |
| G: -4681.25164 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10946.01018 HOMO: -6.51168 LUMO: 1.60275 factor:1 | 1 (-0.39285) | -1 | -1 |
| G: -4681.25164 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10945.27218 HOMO: -6.56067 LUMO: 1.63268 factor:1 | -1 (0.34515) | -1 | -1 |
| G: -4681.25164 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10944.48439 HOMO: -6.56883 LUMO: 1.70615 factor:1 | -1 (1.13295) | -1 | -1 |
| G: -4681.25164 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10946.34273 HOMO: -6.77836 LUMO: 1.77962 factor:1 | 1 (-0.72540) | -1 | -1 |
| G: -4681.25164 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10946.53953 HOMO: -6.38923 LUMO: 1.85854 factor:1 | 1 (-0.92219) | -1 | -1 |
| G: -4681.25164 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10946.56861 HOMO: -6.35658 LUMO: 2.16875 factor:1 | 1 (-0.95128) | -1 | -1 |
| G: -4681.25164 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10946.26485 HOMO: -6.83006 LUMO: 2.31025 factor:1 | 1 (-0.64752) | -1 | -1 |
| G: -4681.25164 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10946.28387 HOMO: -6.87087 LUMO: 1.79051 factor:1 | 1 (-0.66654) | -1 | -1 |
| G: -4681.25164 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10946.93480 HOMO: -6.56339 LUMO: 2.37828 factor:1 | 1 (-1.31747) | -1 | -1 |
| G: -4681.25164 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10946.35517 HOMO: -6.30488 LUMO: 2.51705 factor:1 | 1 (-0.73784) | -1 | -1 |
| G: -4681.25164 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10946.37873 HOMO: -6.69400 LUMO: 1.95650 factor:1 | 1 (-0.76140) | -1 | -1 |
| G: -4681.25164 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10946.55259 HOMO: -6.51168 LUMO: 2.03541 factor:1 | 1 (-0.93526) | -1 | -1 |
| G: -4681.25164 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10946.51727 HOMO: -6.30760 LUMO: 1.65173 factor:1 | 1 (-0.89993) | -1 | -1 |
| G: -4681.25164 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10946.51046 HOMO: -6.55250 LUMO: 1.90752 factor:1 | 1 (-0.89313) | -1 | -1 |
| G: -4681.25164 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10946.13299 HOMO: -6.41372 LUMO: 1.76058 factor:1 | 1 (-0.51566) | -1 | -1 |
| G: -4681.25164 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10946.00278 HOMO: -6.23957 LUMO: 2.06534 factor:1 | 1 (-0.38545) | -1 | -1 |
| G: -4681.25164 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10946.49125 HOMO: -6.58243 LUMO: 2.11705 factor:1 | 1 (-0.87392) | -1 | -1 |
| G: -4681.25164 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10946.48750 HOMO: -6.37835 LUMO: 2.09256 factor:1 | 1 (-0.87017) | -1 | -1 |
| G: -4681.25164 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10945.20777 HOMO: -6.50624 LUMO: 2.55787 factor:1 | -1 (0.40956) | -1 | -1 |
| G: -4681.25164 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10946.43125 HOMO: -6.45454 LUMO: 1.87214 factor:1 | 1 (-0.81392) | -1 | -1 |
| G: -4681.25164 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10946.93567 HOMO: -6.53617 LUMO: 1.95650 factor:1 | 1 (-1.31834) | -1 | -1 |
| G: -4681.25164 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10945.74778 HOMO: -6.51985 LUMO: 1.71432 factor:1 | 1 (-0.13045) | -1 | -1 |
| G: -4681.25164 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10946.81686 HOMO: -6.75114 LUMO: 1.84493 factor:1 | 1 (-1.19953) | -1 | -1 |
| G: -4681.25164 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10946.46352 HOMO: -6.06270 LUMO: 1.65717 factor:1 | 1 (-0.84619) | -1 | -1 |
| G: -4681.25164 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10946.35979 HOMO: -5.89671 LUMO: 1.71704 factor:1 | 1 (-0.74246) | -1 | -1 |
| G: -4681.25164 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10946.44467 HOMO: -6.18787 LUMO: 1.91840 factor:1 | 1 (-0.82733) | -1 | -1 |
| G: -4681.25164 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10947.03464 HOMO: -6.01644 LUMO: 1.85582 factor:1 | 1 (-1.41731) | -1 | -1 |
| G: -4681.25164 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10946.56853 HOMO: -6.05998 LUMO: 2.33474 factor:1 | 1 (-0.95120) | -1 | -1 |
| G: -4681.25164 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10946.53806 HOMO: -6.05725 LUMO: 2.03541 factor:1 | 1 (-0.92072) | -1 | -1 |
| G: -4681.25164 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10946.08605 HOMO: -6.80829 LUMO: 1.90480 factor:1 | 1 (-0.46872) | -1 | -1 |
| G: -4681.25164 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10946.37375 HOMO: -6.76475 LUMO: 2.20956 factor:1 | 1 (-0.75642) | -1 | -1 |
| G: -4681.25164 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10946.26164 HOMO: -6.29944 LUMO: 1.77962 factor:1 | 1 (-0.64431) | -1 | -1 |
| G: -4681.25164 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10944.35342 HOMO: -6.47359 LUMO: -0.25579 factor:1 | -1 (1.26391) | -1 | -1 |
| G: -4681.25164 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10946.15734 HOMO: -6.57699 LUMO: -0.47348 factor:1 | 1 (-0.54001) | -1 | -1 |
| G: -4681.25164 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10945.31363 HOMO: -7.20830 LUMO: 0.49797 factor:1 | -1 (0.30371) | -1 | -1 |
| G: -4681.25164 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10945.16083 HOMO: -7.49402 LUMO: 0.29933 factor:1 | -1 (0.45650) | -1 | -1 |
| G: -4681.25164 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10945.04570 HOMO: -6.66679 LUMO: -0.58777 factor:1 | -1 (0.57163) | -1 | -1 |
| G: -4681.25164 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10946.28910 HOMO: -6.67767 LUMO: -0.56328 factor:1 | 1 (-0.67177) | -1 | -1 |
| G: -4681.25164 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10946.90750 HOMO: -7.42871 LUMO: 0.35647 factor:1 | 1 (-1.29017) | -1 | -1 |
| G: -4681.25164 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10946.30619 HOMO: -6.56067 LUMO: -0.54423 factor:1 | 1 (-0.68886) | -1 | -1 |
| G: -4681.25164 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10946.06659 HOMO: -6.56339 LUMO: -0.50341 factor:1 | 1 (-0.44926) | -1 | -1 |
| G: -4681.25164 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10946.39765 HOMO: -6.56067 LUMO: -0.48436 factor:1 | 1 (-0.78031) | -1 | -1 |
| G: -4681.25164 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10946.32091 HOMO: -6.73210 LUMO: 1.75241 factor:1 | 1 (-0.70358) | -1 | -1 |
| G: -4681.25164 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10946.28485 HOMO: -6.48175 LUMO: 1.91296 factor:1 | 1 (-0.66752) | -1 | -1 |
| G: -4681.25164 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10946.13982 HOMO: -6.67767 LUMO: 1.70343 factor:1 | 1 (-0.52249) | -1 | -1 |
| G: -4681.25164 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10946.15040 HOMO: -6.37835 LUMO: 1.96466 factor:1 | 1 (-0.53307) | -1 | -1 |
| G: -4681.25164 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10946.35054 HOMO: -6.40828 LUMO: 2.10072 factor:1 | 1 (-0.73321) | -1 | -1 |
| G: -4681.25164 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10946.37370 HOMO: -6.06542 LUMO: 1.92112 factor:1 | 1 (-0.75637) | -1 | -1 |
| G: -4681.25164 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10946.31272 HOMO: -6.90353 LUMO: 1.83133 factor:1 | 1 (-0.69539) | -1 | -1 |
| G: -4681.25164 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10946.10803 HOMO: -6.37019 LUMO: 1.92929 factor:1 | 1 (-0.49070) | -1 | -1 |
| G: -4681.25164 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10946.88282 HOMO: -6.61509 LUMO: 2.11160 factor:1 | 1 (-1.26549) | -1 | -1 |
| G: -4681.25164 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10945.57148 HOMO: -6.82734 LUMO: 1.77146 factor:1 | -1 (0.04585) | -1 | -1 |
| G: -4681.25164 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10945.36699 HOMO: -6.01100 LUMO: 1.89935 factor:1 | -1 (0.25034) | -1 | -1 |
| G: -4681.25164 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10945.85293 HOMO: -6.49536 LUMO: 1.75241 factor:1 | 1 (-0.23560) | -1 | -1 |
| G: -4681.25164 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10946.11908 HOMO: -6.34297 LUMO: 1.86398 factor:1 | 1 (-0.50175) | -1 | -1 |
| G: -4681.25164 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10946.05826 HOMO: -6.53073 LUMO: 1.84493 factor:1 | 1 (-0.44093) | -1 | -1 |
| G: -4681.25164 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10945.25904 HOMO: -6.53345 LUMO: 2.41093 factor:1 | -1 (0.35829) | -1 | -1 |
| G: -4681.25164 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10944.89038 HOMO: -7.01237 LUMO: 2.06262 factor:1 | -1 (0.72695) | -1 | -1 |
| G: -4681.25164 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10945.92792 HOMO: -6.17154 LUMO: 1.89119 factor:1 | 1 (-0.31059) | -1 | -1 |
| G: -4681.25164 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10944.98464 HOMO: -6.08719 LUMO: 1.74425 factor:1 | -1 (0.63269) | -1 | -1 |
| G: -4681.25164 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10946.27187 HOMO: -6.69672 LUMO: 1.95106 factor:1 | 1 (-0.65454) | -1 | -1 |
| G: -4681.25164 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10945.45088 HOMO: -6.58243 LUMO: 2.24766 factor:1 | -1 (0.16645) | -1 | -1 |
| G: -4681.25164 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10946.52954 HOMO: -6.74570 LUMO: 2.02181 factor:1 | 1 (-0.91221) | -1 | -1 |
| G: -4681.25164 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10945.72854 HOMO: -6.53890 LUMO: 1.92929 factor:1 | 1 (-0.11121) | -1 | -1 |
| G: -4681.25164 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10946.41141 HOMO: -6.03276 LUMO: 1.67078 factor:1 | 1 (-0.79408) | -1 | -1 |
| G: -4681.25164 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10946.63033 HOMO: -6.67767 LUMO: 2.03541 factor:1 | 1 (-1.01300) | -1 | -1 |
| G: -4681.25164 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10945.98311 HOMO: -5.98378 LUMO: 1.84221 factor:1 | 1 (-0.36578) | -1 | -1 |
| G: -4681.25164 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10945.57891 HOMO: -6.07086 LUMO: 2.01908 factor:1 | -1 (0.03842) | -1 | -1 |
| G: -4681.25164 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10946.47248 HOMO: -6.29944 LUMO: 1.90208 factor:1 | 1 (-0.85515) | -1 | -1 |
| G: -4681.25164 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10946.31669 HOMO: -6.75114 LUMO: 1.85854 factor:1 | 1 (-0.69936) | -1 | -1 |
| G: -4681.25164 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10946.51392 HOMO: -6.56611 LUMO: 2.49801 factor:1 | 1 (-0.89659) | -1 | -1 |
| G: -4681.25164 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10946.55667 HOMO: -6.39740 LUMO: 1.92929 factor:1 | 1 (-0.93934) | -1 | -1 |
| G: -4681.25164 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10946.39310 HOMO: -6.85999 LUMO: -1.07757 factor:1 | 1 (-0.77577) | -1 | -1 |
| G: -4681.25164 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10946.38458 HOMO: -6.98244 LUMO: 1.07213 factor:1 | 1 (-0.76725) | -1 | -1 |
| G: -4681.25164 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10946.12194 HOMO: -7.04231 LUMO: 0.64219 factor:1 | 1 (-0.50461) | -1 | -1 |
| G: -4681.25164 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10944.38542 HOMO: -6.96339 LUMO: 0.75648 factor:1 | -1 (1.23191) | -1 | -1 |
| G: -4681.25164 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10946.16039 HOMO: -6.83822 LUMO: -0.97417 factor:1 | 1 (-0.54306) | -1 | -1 |
| G: -4681.25164 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10946.15772 HOMO: -6.44910 LUMO: -2.15242 factor:1 | 1 (-0.54039) | -1 | -1 |
| G: -4681.25164 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10946.49650 HOMO: -6.84094 LUMO: -1.37690 factor:1 | 1 (-0.87917) | -1 | -1 |
| G: -4681.25164 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10946.57237 HOMO: -6.74026 LUMO: -2.54699 factor:1 | 1 (-0.95504) | -1 | -1 |
| G: -4681.25164 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10946.07369 HOMO: -6.96611 LUMO: 1.24900 factor:1 | 1 (-0.45636) | -1 | -1 |
| G: -4681.25164 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10946.55746 HOMO: -7.21102 LUMO: 0.82995 factor:1 | 1 (-0.94013) | -1 | -1 |
| G: -4681.25164 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10946.60530 HOMO: -6.88448 LUMO: 0.81634 factor:1 | 1 (-0.98796) | -1 | -1 |
| G: -4681.25164 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10944.16764 HOMO: -7.04231 LUMO: 1.10750 factor:1 | -1 (1.44969) | -1 | -1 |
| G: -4681.25164 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10946.44671 HOMO: -6.83550 LUMO: -0.98777 factor:1 | 1 (-0.82938) | -1 | -1 |
| G: -4681.25164 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10946.14798 HOMO: -6.82189 LUMO: 0.93879 factor:1 | 1 (-0.53065) | -1 | -1 |
| G: -4681.25164 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10946.53846 HOMO: -6.81101 LUMO: 0.70750 factor:1 | 1 (-0.92113) | -1 | -1 |
| G: -4681.25164 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10946.24205 HOMO: -7.06680 LUMO: 0.74015 factor:1 | 1 (-0.62472) | -1 | -1 |
| G: -4681.25164 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10946.13633 HOMO: -6.68856 LUMO: 0.86260 factor:1 | 1 (-0.51900) | -1 | -1 |
| G: -4681.25164 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10945.97070 HOMO: -6.83822 LUMO: -0.63403 factor:1 | 1 (-0.35337) | -1 | -1 |
| G: -4681.25164 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10945.81897 HOMO: -6.84911 LUMO: 1.26533 factor:1 | 1 (-0.20164) | -1 | -1 |
| G: -4681.25164 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10945.21803 HOMO: -7.01237 LUMO: 0.73743 factor:1 | -1 (0.39930) | -1 | -1 |
| G: -4681.25164 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10946.00645 HOMO: -7.00965 LUMO: 1.40139 factor:1 | 1 (-0.38912) | -1 | -1 |
| G: -4681.25164 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10945.13934 HOMO: -6.73210 LUMO: -2.49256 factor:1 | -1 (0.47800) | -1 | -1 |
| G: -4681.25164 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10946.21035 HOMO: -7.08040 LUMO: 0.84627 factor:1 | 1 (-0.59302) | -1 | -1 |
| G: -4681.25164 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10945.23379 HOMO: -7.00965 LUMO: 0.82995 factor:1 | -1 (0.38354) | -1 | -1 |
| G: -4681.25164 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10945.95807 HOMO: -6.88448 LUMO: 0.82723 factor:1 | 1 (-0.34074) | -1 | -1 |
| G: -4681.25164 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10944.99484 HOMO: -7.20013 LUMO: 0.88437 factor:1 | -1 (0.62249) | -1 | -1 |
| G: -4681.25164 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10945.16396 HOMO: -6.60420 LUMO: -0.53334 factor:1 | -1 (0.45337) | -1 | -1 |
| G: -4681.25164 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10945.44340 HOMO: -6.78652 LUMO: -0.79729 factor:1 | -1 (0.17394) | -1 | -1 |
| G: -4681.25164 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10946.34736 HOMO: -6.48992 LUMO: -0.64491 factor:1 | 1 (-0.73003) | -1 | -1 |
| G: -4681.25164 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10946.09690 HOMO: -6.85999 LUMO: -0.78097 factor:1 | 1 (-0.47957) | -1 | -1 |
| G: -4681.25164 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10946.75153 HOMO: -6.65046 LUMO: -0.78097 factor:1 | 1 (-1.13420) | -1 | -1 |
| G: -4681.25164 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10946.35705 HOMO: -7.24095 LUMO: 0.37280 factor:1 | 1 (-0.73971) | -1 | -1 |
| G: -4681.25164 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10946.80636 HOMO: -6.81101 LUMO: -0.74831 factor:1 | 1 (-1.18903) | -1 | -1 |
| G: -4681.25164 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10946.06278 HOMO: -6.69400 LUMO: -0.77280 factor:1 | 1 (-0.44545) | -1 | -1 |
| G: -4681.25164 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10946.07228 HOMO: -6.08447 LUMO: -0.68573 factor:1 | 1 (-0.45495) | -1 | -1 |
| G: -4681.25164 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10946.20145 HOMO: -6.66679 LUMO: -0.47076 factor:1 | 1 (-0.58412) | -1 | -1 |
| G: -4681.25164 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10946.02762 HOMO: -6.97428 LUMO: -1.10750 factor:1 | 1 (-0.41029) | -1 | -1 |
| G: -4681.25164 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10945.44084 HOMO: -6.69128 LUMO: -0.54151 factor:1 | -1 (0.17649) | -1 | -1 |
| G: -4681.25164 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10945.84433 HOMO: -6.53617 LUMO: -0.35375 factor:1 | 1 (-0.22700) | -1 | -1 |
| G: -4681.25164 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10945.66242 HOMO: -6.75659 LUMO: -0.41361 factor:1 | 1 (-0.04509) | -1 | -1 |
| G: -4681.25164 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10944.35083 HOMO: -6.69400 LUMO: -0.67484 factor:1 | -1 (1.26650) | -1 | -1 |
| G: -4681.25164 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10944.36300 HOMO: -6.89264 LUMO: -0.90886 factor:1 | -1 (1.25434) | -1 | -1 |
| G: -4681.25164 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10946.10735 HOMO: -6.56339 LUMO: -0.52518 factor:1 | 1 (-0.49002) | -1 | -1 |
| G: -4681.25164 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10945.31281 HOMO: -6.45726 LUMO: -0.65852 factor:1 | -1 (0.30452) | -1 | -1 |
| G: -4681.25164 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10945.35066 HOMO: -6.80557 LUMO: -0.56600 factor:1 | -1 (0.26667) | -1 | -1 |
| G: -4681.25164 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10944.92869 HOMO: -7.19469 LUMO: -0.91702 factor:1 | -1 (0.68864) | -1 | -1 |
| G: -4681.25164 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10944.81272 HOMO: -6.41100 LUMO: 0.79185 factor:1 | -1 (0.80461) | -1 | -1 |
| G: -4681.25164 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10946.00112 HOMO: -6.39195 LUMO: 0.26123 factor:1 | 1 (-0.38379) | -1 | -1 |
| G: -4681.25164 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10944.80262 HOMO: -6.78924 LUMO: 0.35919 factor:1 | -1 (0.81471) | -1 | -1 |
| G: -4681.25164 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10946.48344 HOMO: -6.50624 LUMO: 0.71838 factor:1 | 1 (-0.86611) | -1 | -1 |
| G: -4681.25164 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10946.29359 HOMO: -6.68584 LUMO: -0.66124 factor:1 | 1 (-0.67626) | -1 | -1 |
| G: -4681.25164 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10946.28828 HOMO: -6.45182 LUMO: -0.48980 factor:1 | 1 (-0.67095) | -1 | -1 |
| G: -4681.25164 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10946.11054 HOMO: -7.18925 LUMO: -1.01498 factor:1 | 1 (-0.49321) | -1 | -1 |
| G: -4681.25164 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10944.01224 HOMO: -7.18925 LUMO: -0.63130 factor:1 | -1 (1.60509) | -1 | -1 |
| G: -4681.25164 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10944.24612 HOMO: -6.66679 LUMO: -0.57960 factor:1 | -1 (1.37121) | -1 | -1 |
| G: -4681.25164 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10944.47307 HOMO: -6.44910 LUMO: -0.30205 factor:1 | -1 (1.14427) | -1 | -1 |
| G: -4681.25164 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10944.15994 HOMO: -7.23279 LUMO: 0.46804 factor:1 | -1 (1.45739) | -1 | -1 |
| G: -4681.25164 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10944.33690 HOMO: -6.92802 LUMO: -0.72927 factor:1 | -1 (1.28043) | -1 | -1 |
| G: -4681.25164 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10944.44311 HOMO: -6.83278 LUMO: -0.59321 factor:1 | -1 (1.17423) | -1 | -1 |
| G: -4681.25164 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10944.16675 HOMO: -7.44776 LUMO: 0.27211 factor:1 | -1 (1.45058) | -1 | -1 |
| G: -4681.25164 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10944.00201 HOMO: -6.80829 LUMO: -0.59865 factor:1 | -1 (1.61532) | -1 | -1 |
| G: -4681.25164 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10944.37056 HOMO: -6.63686 LUMO: -0.75103 factor:1 | -1 (1.24677) | -1 | -1 |
| G: -4681.25164 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10944.06171 HOMO: -6.73210 LUMO: -0.55511 factor:1 | -1 (1.55562) | -1 | -1 |
| G: -4681.25164 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10944.35140 HOMO: -6.50624 LUMO: 1.58642 factor:1 | -1 (1.26593) | -1 | -1 |
| G: -4681.25164 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10945.21947 HOMO: -6.79196 LUMO: 0.96328 factor:1 | -1 (0.39786) | -1 | -1 |
| G: -4681.25164 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10945.03185 HOMO: -6.82734 LUMO: 1.23540 factor:1 | -1 (0.58548) | -1 | -1 |
| G: -4681.25164 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10944.85383 HOMO: -6.90081 LUMO: 1.25444 factor:1 | -1 (0.76350) | -1 | -1 |
| G: -4681.25164 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10944.72289 HOMO: -7.00965 LUMO: -1.05036 factor:1 | -1 (0.89444) | -1 | -1 |
| G: -4681.25164 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10945.01139 HOMO: -7.01237 LUMO: -1.48302 factor:1 | -1 (0.60594) | -1 | -1 |
| G: -4681.25164 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10944.82137 HOMO: -6.91713 LUMO: 0.93607 factor:1 | -1 (0.79596) | -1 | -1 |
| G: -4681.25164 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10946.00327 HOMO: -7.02598 LUMO: 0.92247 factor:1 | 1 (-0.38594) | -1 | -1 |
| G: -4681.25164 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10945.06951 HOMO: -6.98516 LUMO: 1.52384 factor:1 | -1 (0.54782) | -1 | -1 |
| G: -4681.25164 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10945.78580 HOMO: -6.75387 LUMO: 1.04764 factor:1 | 1 (-0.16847) | -1 | -1 |
| G: -4681.25164 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10944.91280 HOMO: -7.09401 LUMO: 1.19458 factor:1 | -1 (0.70453) | -1 | -1 |
| G: -4681.25164 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10946.00841 HOMO: -6.88992 LUMO: -1.56193 factor:1 | 1 (-0.39108) | -1 | -1 |
| G: -4681.25164 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10945.13988 HOMO: -7.00149 LUMO: 0.99866 factor:1 | -1 (0.47745) | -1 | -1 |
| G: -4681.25164 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10943.87207 HOMO: -7.13755 LUMO: 1.05308 factor:1 | -1 (1.74526) | -1 | -1 |
| G: -4681.25164 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10944.02762 HOMO: -6.85183 LUMO: -1.42860 factor:1 | -1 (1.58972) | -1 | -1 |
| G: -4681.25164 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10943.96364 HOMO: -6.63141 LUMO: -0.88981 factor:1 | -1 (1.65369) | -1 | -1 |
| G: -4681.25164 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10943.97074 HOMO: -6.92258 LUMO: -0.82178 factor:1 | -1 (1.64659) | -1 | -1 |
| G: -4681.25164 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10943.81343 HOMO: -6.55794 LUMO: -0.80818 factor:1 | -1 (1.80390) | -1 | -1 |
| G: -4681.25164 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10943.98500 HOMO: -6.95251 LUMO: -0.97145 factor:1 | -1 (1.63233) | -1 | -1 |
| G: -4681.25164 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10944.22065 HOMO: -7.37701 LUMO: 0.14150 factor:1 | -1 (1.39668) | -1 | -1 |
| G: -4681.25164 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10944.00059 HOMO: -6.74842 LUMO: -0.68028 factor:1 | -1 (1.61674) | -1 | -1 |
| G: -4681.25164 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10944.10988 HOMO: -6.65046 LUMO: -0.52518 factor:1 | -1 (1.50746) | -1 | -1 |
| G: -4681.25164 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10944.19989 HOMO: -6.91441 LUMO: -1.13199 factor:1 | -1 (1.41744) | -1 | -1 |
| G: -4681.25164 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10944.25012 HOMO: -7.00965 LUMO: -1.00682 factor:1 | -1 (1.36721) | -1 | -1 |
| G: -4681.25164 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10944.33831 HOMO: -6.55794 LUMO: -0.54967 factor:1 | -1 (1.27902) | -1 | -1 |
| G: -5117.60809 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11379.05308 HOMO: -6.71577 LUMO: -0.53879 factor:1 | -1 (2.92071) | -1 | -1 |
| G: -5117.60809 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11383.15601 HOMO: -6.88992 LUMO: -0.55511 factor:1 | 1 (-1.18223) | -1 | -1 |
| G: -5117.60809 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11383.52443 HOMO: -6.74026 LUMO: -0.60681 factor:1 | 1 (-1.55064) | -1 | -1 |
| G: -5117.60809 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11383.42954 HOMO: -6.76747 LUMO: -0.50885 factor:1 | 1 (-1.45575) | -1 | -1 |
| G: -5117.60809 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11383.14295 HOMO: -6.87904 LUMO: -0.92519 factor:1 | 1 (-1.16916) | -1 | -1 |
| G: -5117.60809 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11383.15993 HOMO: -6.53073 LUMO: -0.53062 factor:1 | 1 (-1.18614) | -1 | -1 |
| G: -5117.60809 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11383.29027 HOMO: -6.97700 LUMO: -0.98505 factor:1 | 1 (-1.31649) | -1 | -1 |
| G: -5117.60809 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11382.78087 HOMO: -6.96884 LUMO: -0.79185 factor:1 | 1 (-0.80709) | -1 | -1 |
| G: -5117.60809 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11383.21952 HOMO: -6.60420 LUMO: -0.31021 factor:1 | 1 (-1.24574) | -1 | -1 |
| G: -5117.60809 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11383.38840 HOMO: -6.68584 LUMO: -0.63947 factor:1 | 1 (-1.41461) | -1 | -1 |
| G: -5117.60809 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11383.20962 HOMO: -6.41917 LUMO: -0.35103 factor:1 | 1 (-1.23583) | -1 | -1 |
| G: -5117.60809 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11383.22219 HOMO: -6.73482 LUMO: -0.70477 factor:1 | 1 (-1.24840) | -1 | -1 |
| G: -5220.16791 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11486.58627 HOMO: -6.71305 LUMO: -0.85716 factor:1 | 1 (-2.05266) | -1 | -1 |
| G: -5220.16791 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11486.75923 HOMO: -6.70761 LUMO: -0.63403 factor:1 | 1 (-2.22562) | -1 | -1 |
| G: -5220.16791 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11487.15308 HOMO: -6.37563 LUMO: -0.38640 factor:1 | 1 (-2.61948) | -1 | -1 |
| G: -5220.16791 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11486.97923 HOMO: -6.27495 LUMO: -0.54967 factor:1 | 1 (-2.44562) | -1 | -1 |
| G: -5220.16791 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11486.85732 HOMO: -6.98516 LUMO: 0.38096 factor:1 | 1 (-2.32372) | -1 | -1 |
| G: -5220.16791 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11486.39557 HOMO: -6.47087 LUMO: -0.40001 factor:1 | 1 (-1.86197) | -1 | -1 |
| G: -5220.16791 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11486.40793 HOMO: -6.59876 LUMO: 0.20681 factor:1 | 1 (-1.87432) | -1 | -1 |
| G: -5220.16791 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11486.16969 HOMO: -6.89809 LUMO: 0.14966 factor:1 | 1 (-1.63608) | -1 | -1 |
| G: -5220.16791 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11486.52643 HOMO: -6.76203 LUMO: 2.11432 factor:1 | 1 (-1.99283) | -1 | -1 |
| G: -5220.16791 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11486.72929 HOMO: -6.58516 LUMO: 1.75786 factor:1 | 1 (-2.19569) | -1 | -1 |
| G: -5220.16791 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11487.42395 HOMO: -6.37835 LUMO: 1.84493 factor:1 | 1 (-2.89034) | -1 | -1 |
| G: -5220.16791 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11485.77646 HOMO: -6.83550 LUMO: 1.74425 factor:1 | 1 (-1.24285) | -1 | -1 |
| G: -5220.16791 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11485.38521 HOMO: -6.65318 LUMO: 1.79051 factor:1 | 1 (-0.85161) | -1 | -1 |
| G: -5220.16791 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11486.48747 HOMO: -6.68584 LUMO: 2.11160 factor:1 | 1 (-1.95386) | -1 | -1 |
| G: -5220.16791 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11487.40114 HOMO: -6.36202 LUMO: 1.85037 factor:1 | 1 (-2.86754) | -1 | -1 |
| G: -5220.16791 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11486.68214 HOMO: -6.68312 LUMO: 2.23133 factor:1 | 1 (-2.14853) | -1 | -1 |
| G: -5220.16791 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11487.36895 HOMO: -6.66679 LUMO: 2.14154 factor:1 | 1 (-2.83534) | -1 | -1 |
| G: -5220.16791 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11486.61340 HOMO: -6.50896 LUMO: 1.92657 factor:1 | 1 (-2.07979) | -1 | -1 |
| G: -5220.16791 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11487.38936 HOMO: -6.63686 LUMO: 2.22317 factor:1 | 1 (-2.85575) | -1 | -1 |
| G: -5220.16791 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11485.60318 HOMO: -6.58788 LUMO: 2.17419 factor:1 | 1 (-1.06957) | -1 | -1 |
| G: -5220.16791 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11485.53610 HOMO: -6.72665 LUMO: 2.12249 factor:1 | 1 (-1.00249) | -1 | -1 |
| G: -5220.16791 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11486.89819 HOMO: -6.28311 LUMO: 1.91024 factor:1 | 1 (-2.36459) | -1 | -1 |
| G: -5220.16791 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11486.07666 HOMO: -6.56067 LUMO: 2.27487 factor:1 | 1 (-1.54305) | -1 | -1 |
| G: -5220.16791 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11486.25426 HOMO: -6.83006 LUMO: 2.28031 factor:1 | 1 (-1.72066) | -1 | -1 |
| G: -5220.16791 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11487.21390 HOMO: -6.45182 LUMO: 1.62724 factor:1 | 1 (-2.68029) | -1 | -1 |
| G: -5220.16791 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11486.99640 HOMO: -6.78380 LUMO: 1.83677 factor:1 | 1 (-2.46279) | -1 | -1 |
| G: -5220.16791 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11485.46369 HOMO: -6.23413 LUMO: 1.80956 factor:1 | 1 (-0.93009) | -1 | -1 |
| G: -5220.16791 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11486.26286 HOMO: -6.74298 LUMO: 2.16875 factor:1 | 1 (-1.72926) | -1 | -1 |
| G: -5220.16791 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11485.41400 HOMO: -6.81645 LUMO: 2.50073 factor:1 | 1 (-0.88040) | -1 | -1 |
| G: -5220.16791 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11485.11253 HOMO: -6.71033 LUMO: 1.96466 factor:1 | 1 (-0.57892) | -1 | -1 |
| G: -5220.16791 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11486.11736 HOMO: -6.83550 LUMO: 2.04358 factor:1 | 1 (-1.58376) | -1 | -1 |
| G: -5220.16791 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11485.70419 HOMO: -6.60965 LUMO: 2.38100 factor:1 | 1 (-1.17058) | -1 | -1 |
| G: -5220.16791 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11487.24547 HOMO: -6.73210 LUMO: 2.26127 factor:1 | 1 (-2.71186) | -1 | -1 |
| G: -5220.16791 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11486.86339 HOMO: -6.76203 LUMO: 2.13609 factor:1 | 1 (-2.32978) | -1 | -1 |
| G: -5220.16791 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11486.09399 HOMO: -6.71033 LUMO: 2.05990 factor:1 | 1 (-1.56038) | -1 | -1 |
| G: -5220.16791 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11485.66408 HOMO: -6.50896 LUMO: 2.32385 factor:1 | 1 (-1.13047) | -1 | -1 |
| G: -5220.16791 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11486.46208 HOMO: -6.53345 LUMO: 1.74425 factor:1 | 1 (-1.92847) | -1 | -1 |
| G: -5220.16791 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11486.86075 HOMO: -6.25862 LUMO: 1.63540 factor:1 | 1 (-2.32714) | -1 | -1 |
| G: -5220.16791 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11486.65223 HOMO: -5.90759 LUMO: 1.78779 factor:1 | 1 (-2.11862) | -1 | -1 |
| G: -5220.16791 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11486.03325 HOMO: -6.09807 LUMO: 1.99732 factor:1 | 1 (-1.49965) | -1 | -1 |
| G: -5220.16791 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11486.20909 HOMO: -5.92392 LUMO: 1.99732 factor:1 | 1 (-1.67549) | -1 | -1 |
| G: -5220.16791 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11487.04636 HOMO: -6.45182 LUMO: 1.72248 factor:1 | 1 (-2.51275) | -1 | -1 |
| G: -5220.16791 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11486.39846 HOMO: -6.53073 LUMO: 1.82588 factor:1 | 1 (-1.86485) | -1 | -1 |
| G: -5220.16791 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11486.65237 HOMO: -6.40828 LUMO: 2.05174 factor:1 | 1 (-2.11876) | -1 | -1 |
| G: -5220.16791 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11487.41888 HOMO: -6.60420 LUMO: -0.82450 factor:1 | 1 (-2.88528) | -1 | -1 |
| G: -5220.16791 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11486.34507 HOMO: -6.76747 LUMO: -0.57144 factor:1 | 1 (-1.81146) | -1 | -1 |
| G: -5220.16791 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11486.65816 HOMO: -6.67767 LUMO: -0.59321 factor:1 | 1 (-2.12456) | -1 | -1 |
| G: -5220.16791 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11486.45645 HOMO: -6.65863 LUMO: -0.57416 factor:1 | 1 (-1.92284) | -1 | -1 |
| G: -5220.16791 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11486.79716 HOMO: -6.49808 LUMO: -0.54695 factor:1 | 1 (-2.26355) | -1 | -1 |
| G: -5220.16791 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11486.82078 HOMO: -6.50080 LUMO: -0.61498 factor:1 | 1 (-2.28717) | -1 | -1 |
| G: -5220.16791 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11485.14086 HOMO: -6.74842 LUMO: -0.51974 factor:1 | 1 (-0.60725) | -1 | -1 |
| G: -5220.16791 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11485.25740 HOMO: -6.13345 LUMO: 0.67756 factor:1 | 1 (-0.72380) | -1 | -1 |
| G: -5220.16791 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11485.14758 HOMO: -6.48719 LUMO: 0.52790 factor:1 | 1 (-0.61397) | -1 | -1 |
| G: -5220.16791 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11485.29700 HOMO: -6.35930 LUMO: 0.74015 factor:1 | 1 (-0.76339) | -1 | -1 |
| G: -5220.16791 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11485.47635 HOMO: -6.41644 LUMO: 0.22313 factor:1 | 1 (-0.94274) | -1 | -1 |
| G: -5220.16791 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11485.46788 HOMO: -6.85727 LUMO: -0.00272 factor:1 | 1 (-0.93428) | -1 | -1 |
| G: -5220.16791 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11486.08338 HOMO: -6.84638 LUMO: 0.24762 factor:1 | 1 (-1.54977) | -1 | -1 |
| G: -5220.16791 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11486.32657 HOMO: -6.66951 LUMO: 0.39184 factor:1 | 1 (-1.79296) | -1 | -1 |
| G: -5220.16791 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11486.22365 HOMO: -6.62597 LUMO: -0.65035 factor:1 | 1 (-1.69004) | -1 | -1 |
| G: -5220.16791 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11486.30814 HOMO: -7.13755 LUMO: 0.45715 factor:1 | 1 (-1.77454) | -1 | -1 |
| G: -5220.16791 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11485.94767 HOMO: -7.12666 LUMO: 0.45171 factor:1 | 1 (-1.41407) | -1 | -1 |
| G: -5220.16791 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11486.53835 HOMO: -6.46270 LUMO: -0.46259 factor:1 | 1 (-2.00474) | -1 | -1 |
| G: -5220.16791 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11486.74464 HOMO: -6.36202 LUMO: -0.29660 factor:1 | 1 (-2.21103) | -1 | -1 |
| G: -5220.16791 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11486.69577 HOMO: -6.28583 LUMO: 0.40545 factor:1 | 1 (-2.16216) | -1 | -1 |
| G: -5220.16791 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11487.27325 HOMO: -6.70761 LUMO: 0.41906 factor:1 | 1 (-2.73964) | -1 | -1 |
| G: -5220.16791 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11487.10884 HOMO: -6.76203 LUMO: -0.60954 factor:1 | 1 (-2.57523) | -1 | -1 |
| G: -5220.16791 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11486.35421 HOMO: -6.85999 LUMO: -0.75103 factor:1 | 1 (-1.82060) | -1 | -1 |
| G: -5220.16791 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11486.82962 HOMO: -7.19741 LUMO: -1.00954 factor:1 | 1 (-2.29602) | -1 | -1 |
| G: -5220.16791 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11486.21990 HOMO: -6.58243 LUMO: -0.33470 factor:1 | 1 (-1.68629) | -1 | -1 |
| G: -5220.16791 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11486.32673 HOMO: -7.22190 LUMO: 0.49253 factor:1 | 1 (-1.79312) | -1 | -1 |
| G: -5220.16791 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11486.46529 HOMO: -7.22462 LUMO: 0.51974 factor:1 | 1 (-1.93168) | -1 | -1 |
| G: -5220.16791 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11486.15932 HOMO: -7.08584 LUMO: -0.68301 factor:1 | 1 (-1.62572) | -1 | -1 |
| G: -5220.16791 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11486.73332 HOMO: -6.68584 LUMO: -0.29660 factor:1 | 1 (-2.19971) | -1 | -1 |
| G: -5220.16791 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11486.08063 HOMO: -6.33753 LUMO: -0.48436 factor:1 | 1 (-1.54702) | -1 | -1 |
| G: -5220.16791 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11486.84353 HOMO: -7.15932 LUMO: 0.55511 factor:1 | 1 (-2.30992) | -1 | -1 |
| G: -5220.16791 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11486.60113 HOMO: -6.57427 LUMO: 2.01908 factor:1 | 1 (-2.06752) | -1 | -1 |
| G: -5220.16791 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11486.24281 HOMO: -6.75659 LUMO: 2.22045 factor:1 | 1 (-1.70920) | -1 | -1 |
| G: -5220.16791 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11487.28503 HOMO: -6.73482 LUMO: 2.20956 factor:1 | 1 (-2.75142) | -1 | -1 |
| G: -5220.16791 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11487.06125 HOMO: -6.74026 LUMO: 1.76602 factor:1 | 1 (-2.52764) | -1 | -1 |
| G: -5220.16791 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11486.02934 HOMO: -6.95523 LUMO: 1.94834 factor:1 | 1 (-1.49573) | -1 | -1 |
| G: -5220.16791 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11486.86641 HOMO: -6.33209 LUMO: 1.87486 factor:1 | 1 (-2.33280) | -1 | -1 |
| G: -5220.16791 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11487.09654 HOMO: -6.71033 LUMO: 2.12521 factor:1 | 1 (-2.56293) | -1 | -1 |
| G: -5220.16791 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11486.11119 HOMO: -6.50080 LUMO: 2.04902 factor:1 | 1 (-1.57758) | -1 | -1 |
| G: -5220.16791 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11486.90454 HOMO: -6.76475 LUMO: 1.94017 factor:1 | 1 (-2.37093) | -1 | -1 |
| G: -5220.16791 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11486.27769 HOMO: -6.53073 LUMO: 2.08983 factor:1 | 1 (-1.74409) | -1 | -1 |
| G: -5220.16791 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11486.11007 HOMO: -6.69944 LUMO: 2.20684 factor:1 | 1 (-1.57646) | -1 | -1 |
| G: -5220.16791 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11486.18607 HOMO: -6.34570 LUMO: 1.80684 factor:1 | 1 (-1.65247) | -1 | -1 |
| G: -5220.16791 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11486.10787 HOMO: -6.78380 LUMO: 1.95922 factor:1 | 1 (-1.57426) | -1 | -1 |
| G: -5220.16791 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11486.30118 HOMO: -6.93618 LUMO: 1.76058 factor:1 | 1 (-1.76757) | -1 | -1 |
| G: -5220.16791 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11485.51942 HOMO: -6.93346 LUMO: 1.79595 factor:1 | 1 (-0.98581) | -1 | -1 |
| G: -5220.16791 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11485.55542 HOMO: -6.29671 LUMO: 1.75241 factor:1 | 1 (-1.02181) | -1 | -1 |
| G: -5220.16791 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11485.62334 HOMO: -6.77019 LUMO: 1.74697 factor:1 | 1 (-1.08973) | -1 | -1 |
| G: -5220.16791 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11485.47401 HOMO: -6.87360 LUMO: 1.91024 factor:1 | 1 (-0.94040) | -1 | -1 |
| G: -5220.16791 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11485.11261 HOMO: -6.32665 LUMO: 1.87759 factor:1 | 1 (-0.57900) | -1 | -1 |
| G: -5220.16791 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11485.42007 HOMO: -6.99877 LUMO: 1.99187 factor:1 | 1 (-0.88647) | -1 | -1 |
| G: -5220.16791 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11486.14836 HOMO: -6.72665 LUMO: 2.12521 factor:1 | 1 (-1.61475) | -1 | -1 |
| G: -5220.16791 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11486.26572 HOMO: -6.67767 LUMO: 2.43814 factor:1 | 1 (-1.73211) | -1 | -1 |
| G: -5220.16791 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11486.07981 HOMO: -6.99605 LUMO: 1.79051 factor:1 | 1 (-1.54621) | -1 | -1 |
| G: -5220.16791 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11485.52799 HOMO: -6.25046 LUMO: 1.77146 factor:1 | 1 (-0.99439) | -1 | -1 |
| G: -5220.16791 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11485.44535 HOMO: -6.30488 LUMO: 1.90480 factor:1 | 1 (-0.91174) | -1 | -1 |
| G: -5220.16791 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11485.32061 HOMO: -6.38379 LUMO: 1.68438 factor:1 | 1 (-0.78701) | -1 | -1 |
| G: -5220.16791 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11485.49776 HOMO: -6.78924 LUMO: 2.01364 factor:1 | 1 (-0.96415) | -1 | -1 |
| G: -5220.16791 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11485.36837 HOMO: -6.15249 LUMO: 1.98643 factor:1 | 1 (-0.83476) | -1 | -1 |
| G: -5220.16791 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11485.17993 HOMO: -6.19331 LUMO: 2.14154 factor:1 | 1 (-0.64632) | -1 | -1 |
| G: -5220.16791 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11486.90342 HOMO: -6.05998 LUMO: 2.12521 factor:1 | 1 (-2.36981) | -1 | -1 |
| G: -5220.16791 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11486.02332 HOMO: -6.67223 LUMO: 1.91840 factor:1 | 1 (-1.48971) | -1 | -1 |
| G: -5220.16791 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11486.17913 HOMO: -6.79196 LUMO: 2.18507 factor:1 | 1 (-1.64553) | -1 | -1 |
| G: -5220.16791 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11486.09764 HOMO: -6.93346 LUMO: 1.78235 factor:1 | 1 (-1.56403) | -1 | -1 |
| G: -5220.16791 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11485.91684 HOMO: -6.16882 LUMO: 1.80956 factor:1 | 1 (-1.38324) | -1 | -1 |
| G: -5220.16791 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11485.98958 HOMO: -6.72665 LUMO: 2.07895 factor:1 | 1 (-1.45597) | -1 | -1 |
| G: -5220.16791 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11485.61899 HOMO: -6.73210 LUMO: 1.97827 factor:1 | 1 (-1.08538) | -1 | -1 |
| G: -5220.16791 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11486.09320 HOMO: -6.84638 LUMO: 1.87214 factor:1 | 1 (-1.55959) | -1 | -1 |
| G: -5220.16791 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11486.21976 HOMO: -6.83006 LUMO: 2.36195 factor:1 | 1 (-1.68615) | -1 | -1 |
| G: -5220.16791 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11486.04523 HOMO: -6.97700 LUMO: 1.91024 factor:1 | 1 (-1.51162) | -1 | -1 |
| G: -5220.16791 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11486.50945 HOMO: -6.20420 LUMO: 1.81772 factor:1 | 1 (-1.97585) | -1 | -1 |
| G: -5220.16791 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11486.26684 HOMO: -7.09129 LUMO: 2.10344 factor:1 | 1 (-1.73323) | 1 | 1 |
| G: -5220.16791 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11484.99027 HOMO: -6.77564 LUMO: 2.14970 factor:1 | 1 (-0.45666) | -1 | -1 |
| G: -5220.16791 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11485.40149 HOMO: -6.81645 LUMO: 1.85854 factor:1 | 1 (-0.86788) | -1 | -1 |
| G: -5220.16791 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11485.21969 HOMO: -6.50896 LUMO: 2.04358 factor:1 | 1 (-0.68608) | -1 | -1 |
| G: -5220.16791 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11485.01835 HOMO: -6.89264 LUMO: 1.66262 factor:1 | 1 (-0.48474) | -1 | -1 |
| G: -5220.16791 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11485.26636 HOMO: -6.75931 LUMO: 2.23950 factor:1 | 1 (-0.73275) | -1 | -1 |
| G: -5220.16791 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11485.47147 HOMO: -6.50080 LUMO: 1.67622 factor:1 | 1 (-0.93787) | -1 | -1 |
| G: -5220.16791 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11485.01089 HOMO: -6.30216 LUMO: 2.24222 factor:1 | 1 (-0.47729) | -1 | -1 |
| G: -5220.16791 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11485.28119 HOMO: -7.18108 LUMO: 2.10072 factor:1 | 1 (-0.74758) | 1 | 1 |
| G: -5220.16791 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11485.48671 HOMO: -6.54162 LUMO: 2.35378 factor:1 | 1 (-0.95311) | -1 | -1 |
| G: -5220.16791 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11485.50707 HOMO: -5.98650 LUMO: 1.48302 factor:1 | 1 (-0.97346) | -1 | -1 |
| G: -5220.16791 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11485.76729 HOMO: -7.15115 LUMO: 2.14970 factor:1 | 1 (-1.23368) | 1 | 1 |
| G: -5220.16791 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11486.35699 HOMO: -6.45454 LUMO: 2.15786 factor:1 | 1 (-1.82338) | -1 | -1 |
| G: -5220.16791 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11485.46141 HOMO: -7.06952 LUMO: 2.14970 factor:1 | 1 (-0.92780) | 1 | 1 |
| G: -5220.16791 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11486.23421 HOMO: -6.93618 LUMO: 1.86942 factor:1 | 1 (-1.70060) | -1 | -1 |
| G: -5220.16791 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11486.28254 HOMO: -6.63141 LUMO: 1.92657 factor:1 | 1 (-1.74893) | -1 | -1 |
| G: -5220.16791 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11486.07720 HOMO: -6.51441 LUMO: -0.44355 factor:1 | 1 (-1.54359) | -1 | -1 |
| G: -5220.16791 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11486.08917 HOMO: -6.82734 LUMO: -1.03131 factor:1 | 1 (-1.55557) | -1 | -1 |
| G: -5220.16791 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11485.24200 HOMO: -6.58788 LUMO: -0.82995 factor:1 | 1 (-0.70839) | -1 | -1 |
| G: -5220.16791 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11485.51458 HOMO: -6.43277 LUMO: -0.40817 factor:1 | 1 (-0.98097) | -1 | -1 |
| G: -5220.16791 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11485.42149 HOMO: -6.78924 LUMO: -0.72110 factor:1 | 1 (-0.88788) | -1 | -1 |
| G: -5220.16791 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11485.48413 HOMO: -7.28177 LUMO: 0.36735 factor:1 | 1 (-0.95052) | -1 | -1 |
| G: -5220.16791 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11486.26760 HOMO: -6.47903 LUMO: -0.46259 factor:1 | 1 (-1.73399) | -1 | -1 |
| G: -5220.16791 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11486.25954 HOMO: -6.67495 LUMO: -0.75376 factor:1 | 1 (-1.72594) | -1 | -1 |
| G: -5220.16791 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11485.85695 HOMO: -6.71033 LUMO: -0.71838 factor:1 | 1 (-1.32334) | -1 | -1 |
| G: -5220.16791 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11485.59208 HOMO: -6.79740 LUMO: -0.79185 factor:1 | 1 (-1.05847) | -1 | -1 |
| G: -5220.16791 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11486.22773 HOMO: -6.08719 LUMO: -0.63675 factor:1 | 1 (-1.69413) | -1 | -1 |
| G: -5220.16791 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11486.31867 HOMO: -6.84094 LUMO: 0.42994 factor:1 | 1 (-1.78507) | -1 | -1 |
| G: -5220.16791 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11485.02134 HOMO: -6.59604 LUMO: 0.25851 factor:1 | 1 (-0.48774) | -1 | -1 |
| G: -5220.16791 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11485.30070 HOMO: -6.82462 LUMO: 0.08708 factor:1 | 1 (-0.76709) | -1 | -1 |
| G: -5220.16791 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11485.46244 HOMO: -6.54706 LUMO: 0.44082 factor:1 | 1 (-0.92883) | -1 | -1 |
| G: -5220.16791 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11485.15261 HOMO: -6.99333 LUMO: 0.32109 factor:1 | 1 (-0.61900) | -1 | -1 |
| G: -5220.16791 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11485.05177 HOMO: -6.29944 LUMO: -0.57144 factor:1 | 1 (-0.51816) | -1 | -1 |
| G: -5220.16791 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11485.73061 HOMO: -6.57699 LUMO: -0.46531 factor:1 | 1 (-1.19700) | -1 | -1 |
| G: -5220.16791 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11485.74008 HOMO: -6.24773 LUMO: -0.53879 factor:1 | 1 (-1.20647) | -1 | -1 |
| G: -5220.16791 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11485.94095 HOMO: -6.96067 LUMO: -0.67212 factor:1 | 1 (-1.40735) | -1 | -1 |
| G: -5220.16791 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11486.03227 HOMO: -7.24095 LUMO: -0.09252 factor:1 | 1 (-1.49867) | -1 | -1 |
| G: -5220.16791 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11485.15811 HOMO: -6.33481 LUMO: -0.46531 factor:1 | 1 (-0.62450) | -1 | -1 |
| G: -5220.16791 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11484.92785 HOMO: -6.43549 LUMO: -0.33198 factor:1 | 1 (-0.39424) | -1 | -1 |
| G: -5220.16791 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11485.24423 HOMO: -6.53073 LUMO: 0.44899 factor:1 | 1 (-0.71063) | -1 | -1 |
| G: -5220.16791 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11485.50854 HOMO: -6.69128 LUMO: 0.47620 factor:1 | 1 (-0.97493) | -1 | -1 |
| G: -5220.16791 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11485.44862 HOMO: -6.65318 LUMO: 0.52246 factor:1 | 1 (-0.91501) | -1 | -1 |
| G: -5220.16791 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11485.42356 HOMO: -6.71305 LUMO: 0.41089 factor:1 | 1 (-0.88995) | -1 | -1 |
| G: -5220.16791 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11485.06105 HOMO: -6.70216 LUMO: 0.19864 factor:1 | 1 (-0.52744) | -1 | -1 |
| G: -5220.16791 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11485.37207 HOMO: -6.41100 LUMO: 0.34558 factor:1 | 1 (-0.83846) | -1 | -1 |
| G: -5220.16791 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11486.14507 HOMO: -7.01237 LUMO: 0.02993 factor:1 | 1 (-1.61146) | -1 | -1 |
| G: -5220.16791 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11486.20425 HOMO: -6.85999 LUMO: 0.18776 factor:1 | 1 (-1.67064) | -1 | -1 |
| G: -5220.16791 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11485.28529 HOMO: -6.62869 LUMO: 0.48708 factor:1 | 1 (-0.75169) | -1 | -1 |
| G: -5220.16791 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11486.67933 HOMO: -6.43821 LUMO: -0.45715 factor:1 | 1 (-2.14573) | -1 | -1 |
| G: -5220.16791 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11486.49789 HOMO: -6.43277 LUMO: -0.72110 factor:1 | 1 (-1.96428) | -1 | -1 |
| G: -5220.16791 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11485.70057 HOMO: -7.10761 LUMO: 0.43266 factor:1 | 1 (-1.16696) | -1 | -1 |
| G: -5220.16791 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11486.72921 HOMO: -6.57699 LUMO: -0.61498 factor:1 | 1 (-2.19561) | -1 | -1 |
| G: -5220.16791 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11485.91619 HOMO: -6.82189 LUMO: -0.75648 factor:1 | 1 (-1.38258) | -1 | -1 |
| G: -5220.16791 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11486.04017 HOMO: -6.55794 LUMO: -0.67212 factor:1 | 1 (-1.50656) | -1 | -1 |
| G: -5220.16791 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11485.08257 HOMO: -6.69128 LUMO: 1.88575 factor:1 | 1 (-0.54896) | -1 | -1 |
| G: -5220.16791 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11485.19958 HOMO: -6.65591 LUMO: 1.70888 factor:1 | 1 (-0.66597) | -1 | -1 |
| G: -5220.16791 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11485.82775 HOMO: -6.58788 LUMO: 1.68438 factor:1 | 1 (-1.29415) | -1 | -1 |
| G: -5220.16791 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11485.73121 HOMO: -6.46270 LUMO: 1.72520 factor:1 | 1 (-1.19760) | -1 | -1 |
| G: -5220.16791 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11486.12128 HOMO: -6.57427 LUMO: 1.73881 factor:1 | 1 (-1.58768) | -1 | -1 |
| G: -5220.16791 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11485.87997 HOMO: -6.45182 LUMO: 1.75241 factor:1 | 1 (-1.34636) | -1 | -1 |
| G: -5220.16791 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11485.91614 HOMO: -6.51441 LUMO: 1.78779 factor:1 | 1 (-1.38253) | -1 | -1 |
| G: -5220.16791 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11485.98242 HOMO: -6.67495 LUMO: 2.11705 factor:1 | 1 (-1.44882) | -1 | -1 |
| G: -5220.16791 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11484.96115 HOMO: -6.22597 LUMO: 1.96466 factor:1 | 1 (-0.42755) | -1 | -1 |
| G: -5220.16791 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11485.09310 HOMO: -6.68040 LUMO: 2.30753 factor:1 | 1 (-0.55949) | -1 | -1 |
| G: -5220.16791 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11485.02809 HOMO: -6.65046 LUMO: 2.18235 factor:1 | 1 (-0.49449) | -1 | -1 |
| G: -5220.16791 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11484.99038 HOMO: -6.38651 LUMO: 1.76874 factor:1 | 1 (-0.45677) | -1 | -1 |
| G: -5220.16791 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11484.64847 HOMO: -6.41644 LUMO: 2.09256 factor:1 | 1 (-0.11486) | -1 | -1 |
| G: -5220.16791 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11485.22772 HOMO: -6.14977 LUMO: 2.28031 factor:1 | 1 (-0.69411) | -1 | -1 |
| G: -5220.16791 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11484.98866 HOMO: -6.70489 LUMO: 2.43814 factor:1 | 1 (-0.45506) | -1 | -1 |
| G: -5220.16791 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11485.24453 HOMO: -6.78924 LUMO: 2.27215 factor:1 | 1 (-0.71092) | -1 | -1 |
| G: -5220.16791 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11486.09995 HOMO: -6.86271 LUMO: 2.31025 factor:1 | 1 (-1.56634) | -1 | -1 |
| G: -5220.16791 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11485.74772 HOMO: -6.51168 LUMO: 2.04630 factor:1 | 1 (-1.21412) | -1 | -1 |
| G: -5220.16791 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11486.19108 HOMO: -6.72665 LUMO: 2.13337 factor:1 | 1 (-1.65747) | -1 | -1 |
| G: -5220.16791 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11485.89050 HOMO: -6.45998 LUMO: 2.16058 factor:1 | 1 (-1.35690) | -1 | -1 |
| G: -5220.16791 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11486.04343 HOMO: -6.83822 LUMO: 2.20684 factor:1 | 1 (-1.50982) | -1 | -1 |
| G: -5220.16791 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11485.09275 HOMO: -6.68856 LUMO: 2.19324 factor:1 | 1 (-0.55914) | -1 | -1 |
| G: -5220.16791 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11485.29172 HOMO: -6.71577 LUMO: 2.16058 factor:1 | 1 (-0.75811) | -1 | -1 |
| G: -5220.16791 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11485.35814 HOMO: -6.82462 LUMO: 1.90208 factor:1 | 1 (-0.82453) | -1 | -1 |
| G: -5220.16791 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11485.47586 HOMO: -6.61509 LUMO: 2.23950 factor:1 | 1 (-0.94225) | -1 | -1 |
| G: -5220.16791 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11485.46190 HOMO: -6.73754 LUMO: 1.84221 factor:1 | 1 (-0.92829) | -1 | -1 |
| G: -5220.16791 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11485.62315 HOMO: -6.56611 LUMO: 1.94561 factor:1 | 1 (-1.08954) | -1 | -1 |
| G: -5658.42769 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11921.68578 HOMO: -6.67767 LUMO: 1.51840 factor:1 | -1 (1.10761) | -1 | -1 |
| G: -5658.42769 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11921.91862 HOMO: -6.35658 LUMO: 2.16603 factor:1 | -1 (0.87476) | -1 | -1 |
| G: -5658.42769 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11924.08152 HOMO: -6.35114 LUMO: 2.08983 factor:1 | 1 (-1.28813) | -1 | -1 |
| G: -5658.42769 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11924.27491 HOMO: -6.35114 LUMO: 2.10616 factor:1 | 1 (-1.48152) | -1 | -1 |
| G: -5658.42769 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11924.15453 HOMO: -6.71305 LUMO: 2.01636 factor:1 | 1 (-1.36114) | -1 | -1 |
| G: -5658.42769 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11924.46776 HOMO: -6.24773 LUMO: 1.98915 factor:1 | 1 (-1.67437) | -1 | -1 |
| G: -5658.42769 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11924.49644 HOMO: -6.53617 LUMO: 2.42726 factor:1 | 1 (-1.70305) | -1 | -1 |
| G: -5658.42769 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11923.94312 HOMO: -6.59332 LUMO: 1.82316 factor:1 | 1 (-1.14974) | -1 | -1 |
| G: -5658.42769 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11924.05673 HOMO: -6.41372 LUMO: 1.77418 factor:1 | 1 (-1.26334) | -1 | -1 |
| G: -5658.42769 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11924.13262 HOMO: -6.40284 LUMO: 1.88575 factor:1 | 1 (-1.33924) | -1 | -1 |
| G: -5658.42769 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11924.10098 HOMO: -6.11168 LUMO: 1.70888 factor:1 | 1 (-1.30759) | -1 | -1 |
| G: -5658.42769 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11923.67670 HOMO: -6.44910 LUMO: 2.23405 factor:1 | 1 (-0.88331) | -1 | -1 |
| G: -5658.42769 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11924.31377 HOMO: -6.24773 LUMO: 2.12793 factor:1 | 1 (-1.52038) | -1 | -1 |
| G: -5658.42769 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11923.72981 HOMO: -6.07358 LUMO: 1.89663 factor:1 | 1 (-0.93643) | -1 | -1 |
| G: -5658.42769 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11923.78886 HOMO: -6.66679 LUMO: 1.96738 factor:1 | 1 (-0.99547) | -1 | -1 |
| G: -5658.42769 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11923.89406 HOMO: -6.68312 LUMO: 1.78235 factor:1 | 1 (-1.10067) | -1 | -1 |
| G: -5658.42769 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11923.77490 HOMO: -6.70761 LUMO: 1.97555 factor:1 | 1 (-0.98151) | -1 | -1 |
| G: -5658.42769 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11923.87869 HOMO: -6.15794 LUMO: 2.00548 factor:1 | 1 (-1.08530) | -1 | -1 |
| G: -5658.42769 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11923.99496 HOMO: -6.52257 LUMO: 1.96738 factor:1 | 1 (-1.20157) | -1 | -1 |
| G: -5658.42769 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11924.00848 HOMO: -6.25590 LUMO: 1.86670 factor:1 | 1 (-1.21510) | -1 | -1 |
| G: -5658.42769 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11924.16773 HOMO: -6.30216 LUMO: 1.84765 factor:1 | 1 (-1.37434) | -1 | -1 |
| G: -5658.42769 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11924.30302 HOMO: -6.76747 LUMO: 2.20956 factor:1 | 1 (-1.50963) | -1 | -1 |
| G: -5658.42769 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11924.21986 HOMO: -6.14161 LUMO: 1.80684 factor:1 | 1 (-1.42648) | -1 | -1 |
| G: -5658.42769 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11924.26177 HOMO: -6.81373 LUMO: 1.91024 factor:1 | 1 (-1.46838) | -1 | -1 |
| G: -5658.42769 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11923.99387 HOMO: -6.81917 LUMO: 2.34834 factor:1 | 1 (-1.20048) | -1 | -1 |
| G: -5658.42769 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11923.66600 HOMO: -6.72121 LUMO: 1.90208 factor:1 | 1 (-0.87261) | -1 | -1 |
| G: -5658.42769 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11923.66429 HOMO: -7.51851 LUMO: 0.26939 factor:1 | 1 (-0.87090) | -1 | -1 |
| G: -5658.42769 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11922.72024 HOMO: -6.65318 LUMO: -0.57144 factor:1 | -1 (0.07314) | -1 | -1 |
| G: -5658.42769 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11924.26561 HOMO: -6.77564 LUMO: -0.72654 factor:1 | 1 (-1.47222) | -1 | -1 |
| G: -5658.42769 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11924.23064 HOMO: -6.80557 LUMO: -0.60954 factor:1 | 1 (-1.43725) | -1 | -1 |
| G: -5658.42769 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11923.79912 HOMO: -7.35524 LUMO: 0.27483 factor:1 | 1 (-1.00573) | -1 | -1 |
| G: -5658.42769 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11923.86772 HOMO: -6.94979 LUMO: -0.83811 factor:1 | 1 (-1.07433) | -1 | -1 |
| G: -5658.42769 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11923.69838 HOMO: -6.13345 LUMO: -0.67212 factor:1 | 1 (-0.90500) | -1 | -1 |
| G: -5658.42769 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11922.97312 HOMO: -6.47359 LUMO: -0.59321 factor:1 | 1 (-0.17973) | -1 | -1 |
| G: -5658.42769 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11923.87311 HOMO: -6.52257 LUMO: -0.54695 factor:1 | 1 (-1.07972) | -1 | -1 |
| G: -5658.42769 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11921.93471 HOMO: -6.61781 LUMO: -0.69661 factor:1 | -1 (0.85868) | -1 | -1 |
| G: -5658.42769 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11923.57996 HOMO: -6.77564 LUMO: -0.80001 factor:1 | 1 (-0.78657) | -1 | -1 |
| G: -5658.42769 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11923.99031 HOMO: -7.35252 LUMO: -1.00410 factor:1 | 1 (-1.19692) | -1 | -1 |
| G: -5658.42769 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11924.10144 HOMO: -6.35386 LUMO: -0.38912 factor:1 | 1 (-1.30805) | -1 | -1 |
| G: -6232.52541 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12496.28083 HOMO: -6.80285 LUMO: -0.52246 factor:1 | -1 (0.61027) | -1 | -1 |
| G: -6232.52541 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12496.27218 HOMO: -7.23279 LUMO: 0.30477 factor:1 | -1 (0.61892) | -1 | -1 |
| G: -6231.94940 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12496.28083 HOMO: -7.13483 LUMO: -0.76192 factor:1 | -1 (0.03426) | -1 | -1 |
| G: -6231.94940 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12496.27218 HOMO: -6.71849 LUMO: -0.48164 factor:1 | -1 (0.04291) | -1 | -1 |
| G: -4276.08596 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10541.17962 HOMO: -6.85455 LUMO: -0.69389 factor:1 | 1 (-0.72796) | -1 | -1 |
| G: -4276.08596 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10541.31883 HOMO: -6.96339 LUMO: -0.73743 factor:1 | 1 (-0.86717) | -1 | -1 |
| G: -4276.08596 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10541.07785 HOMO: -7.50490 LUMO: 0.28844 factor:1 | 1 (-0.62619) | -1 | -1 |
| G: -4276.08596 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10541.05439 HOMO: -6.63958 LUMO: -0.50069 factor:1 | 1 (-0.60273) | -1 | -1 |
| G: -4276.08596 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10541.28571 HOMO: -6.78924 LUMO: -0.69661 factor:1 | 1 (-0.83406) | -1 | -1 |
| G: -4276.08596 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10541.01137 HOMO: -7.44776 LUMO: 0.33742 factor:1 | 1 (-0.55971) | -1 | -1 |
| G: -4276.08596 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10541.05447 HOMO: -6.15249 LUMO: 0.66396 factor:1 | 1 (-0.60281) | -1 | -1 |
| G: -4276.08596 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10541.14209 HOMO: -6.17426 LUMO: 0.55511 factor:1 | 1 (-0.69043) | -1 | -1 |
| G: -4276.08596 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10541.21605 HOMO: -6.83550 LUMO: 0.28844 factor:1 | 1 (-0.76440) | -1 | -1 |
| G: -4276.08596 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10540.94843 HOMO: -6.32393 LUMO: 0.47620 factor:1 | 1 (-0.49677) | -1 | -1 |
| G: -4276.08596 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10540.88459 HOMO: -6.32937 LUMO: 0.45987 factor:1 | 1 (-0.43293) | -1 | -1 |
| G: -4276.08596 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10541.09194 HOMO: -7.37429 LUMO: 0.09252 factor:1 | 1 (-0.64028) | -1 | -1 |
| G: -4276.08596 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10541.01839 HOMO: -6.54434 LUMO: -0.39729 factor:1 | 1 (-0.56673) | -1 | -1 |
| G: -4276.08596 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10541.21926 HOMO: -7.35524 LUMO: 0.28028 factor:1 | 1 (-0.76761) | -1 | -1 |
| G: -4276.08596 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10540.97610 HOMO: -6.95523 LUMO: -0.86804 factor:1 | 1 (-0.52445) | -1 | -1 |
| G: -4276.08596 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10540.78287 HOMO: -6.63958 LUMO: -0.65307 factor:1 | 1 (-0.33122) | -1 | -1 |
| G: -4276.08596 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10540.74739 HOMO: -6.73482 LUMO: -0.67212 factor:1 | 1 (-0.29573) | -1 | -1 |
| G: -4276.08596 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10540.63762 HOMO: -6.37835 LUMO: -0.53606 factor:1 | 1 (-0.18596) | -1 | -1 |
| G: -4276.08596 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10541.13523 HOMO: -6.71849 LUMO: -0.61226 factor:1 | 1 (-0.68358) | -1 | -1 |
| G: -4276.08596 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10540.98005 HOMO: -6.68584 LUMO: -1.11022 factor:1 | 1 (-0.52839) | -1 | -1 |
| G: -4276.08596 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10541.31146 HOMO: -6.80285 LUMO: -0.79185 factor:1 | 1 (-0.85980) | -1 | -1 |
| G: -4276.08596 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10540.92524 HOMO: -7.14571 LUMO: -0.94696 factor:1 | 1 (-0.47359) | -1 | -1 |
| G: -4276.08596 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10541.10653 HOMO: -7.16204 LUMO: -0.66124 factor:1 | 1 (-0.65487) | -1 | -1 |
| G: -4276.08596 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10541.26082 HOMO: -6.54978 LUMO: -0.54967 factor:1 | 1 (-0.80916) | -1 | -1 |
| G: -4276.08596 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10541.16179 HOMO: -6.75114 LUMO: -0.70750 factor:1 | 1 (-0.71014) | -1 | -1 |
| G: -4276.08596 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10541.10963 HOMO: -7.22190 LUMO: 0.39184 factor:1 | 1 (-0.65797) | -1 | -1 |
| G: -4276.08596 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10541.10182 HOMO: -7.43959 LUMO: 0.30477 factor:1 | 1 (-0.65016) | -1 | -1 |
| G: -4276.08596 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10541.24307 HOMO: -6.87360 LUMO: -0.77552 factor:1 | 1 (-0.79142) | -1 | -1 |
| G: -4276.08596 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10541.07436 HOMO: -6.82734 LUMO: -0.59593 factor:1 | 1 (-0.62271) | -1 | -1 |
| G: -4276.08596 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10540.97382 HOMO: -6.65318 LUMO: -0.46259 factor:1 | 1 (-0.52216) | -1 | -1 |
| G: -4276.08596 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10540.93950 HOMO: -7.05863 LUMO: -1.17009 factor:1 | 1 (-0.48785) | -1 | -1 |
| G: -4276.08596 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10541.08462 HOMO: -6.57427 LUMO: -0.48708 factor:1 | 1 (-0.63296) | -1 | -1 |
| G: -4276.08596 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10541.01496 HOMO: -6.60420 LUMO: -0.38096 factor:1 | 1 (-0.56330) | -1 | -1 |
| G: -4276.08596 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10541.04239 HOMO: -6.72121 LUMO: -0.66668 factor:1 | 1 (-0.59073) | -1 | -1 |
| G: -4276.08596 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10540.88383 HOMO: -6.52257 LUMO: -0.19320 factor:1 | 1 (-0.43217) | -1 | -1 |
| G: -4276.08596 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10540.72451 HOMO: -6.28039 LUMO: -0.27211 factor:1 | 1 (-0.27285) | -1 | -1 |
| G: -4276.08596 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10540.84464 HOMO: -6.71849 LUMO: -0.42722 factor:1 | 1 (-0.39299) | -1 | -1 |
| G: -4276.08596 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10541.08914 HOMO: -6.27495 LUMO: 0.27756 factor:1 | 1 (-0.63748) | -1 | -1 |
| G: -4276.08596 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10540.86791 HOMO: -6.21780 LUMO: 0.46531 factor:1 | 1 (-0.41625) | -1 | -1 |
| G: -4276.08596 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10540.97390 HOMO: -6.52257 LUMO: -0.64491 factor:1 | 1 (-0.52224) | -1 | -1 |
| G: -4276.08596 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10540.74579 HOMO: -6.73754 LUMO: 1.83133 factor:1 | 1 (-0.29413) | -1 | -1 |
| G: -4276.08596 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10540.71057 HOMO: -6.67223 LUMO: 1.88847 factor:1 | 1 (-0.25892) | -1 | -1 |
| G: -4276.08596 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10540.54782 HOMO: -6.82189 LUMO: 1.59187 factor:1 | 1 (-0.09617) | -1 | -1 |
| G: -4276.08596 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10541.04982 HOMO: -6.43277 LUMO: 1.76330 factor:1 | 1 (-0.59816) | -1 | -1 |
| G: -4276.08596 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10541.00078 HOMO: -6.48175 LUMO: 1.77962 factor:1 | 1 (-0.54913) | -1 | -1 |
| G: -4276.08596 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10541.29954 HOMO: -6.50352 LUMO: 1.68438 factor:1 | 1 (-0.84788) | -1 | -1 |
| G: -4276.08596 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10541.10215 HOMO: -6.31576 LUMO: 2.03813 factor:1 | 1 (-0.65049) | -1 | -1 |
| G: -4276.08596 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10540.86709 HOMO: -6.27495 LUMO: 1.99459 factor:1 | 1 (-0.41544) | -1 | -1 |
| G: -4276.08596 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10540.83743 HOMO: -6.23957 LUMO: 2.17147 factor:1 | 1 (-0.38578) | -1 | -1 |
| G: -4276.08596 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10541.27458 HOMO: -6.78108 LUMO: 2.16875 factor:1 | 1 (-0.82293) | -1 | -1 |
| G: -4276.08596 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10541.14775 HOMO: -6.34297 LUMO: 2.10344 factor:1 | 1 (-0.69609) | -1 | -1 |
| G: -4276.08596 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10540.86576 HOMO: -6.30216 LUMO: 2.00004 factor:1 | 1 (-0.41410) | -1 | -1 |
| G: -4276.08596 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10540.78579 HOMO: -6.72665 LUMO: 2.09528 factor:1 | 1 (-0.33413) | -1 | -1 |
| G: -4276.08596 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10541.14873 HOMO: -6.86543 LUMO: 1.91568 factor:1 | 1 (-0.69707) | -1 | -1 |
| G: -4276.08596 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10540.82222 HOMO: -5.83956 LUMO: 1.89391 factor:1 | 1 (-0.37056) | -1 | -1 |
| G: -4276.08596 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10541.09251 HOMO: -6.42189 LUMO: 2.03269 factor:1 | 1 (-0.64086) | -1 | -1 |
| G: -4276.08596 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10541.06383 HOMO: -6.07630 LUMO: 1.80956 factor:1 | 1 (-0.61217) | -1 | -1 |
| G: -4276.08596 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10541.02122 HOMO: -6.43277 LUMO: 1.81772 factor:1 | 1 (-0.56956) | -1 | -1 |
| G: -4276.08596 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10541.22754 HOMO: -7.03959 LUMO: 1.78779 factor:1 | 1 (-0.77588) | -1 | -1 |
| G: -4276.08596 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10540.75011 HOMO: -6.72121 LUMO: 2.29664 factor:1 | 1 (-0.29845) | -1 | -1 |
| G: -4276.08596 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10540.69800 HOMO: -6.62869 LUMO: 2.04630 factor:1 | 1 (-0.24634) | -1 | -1 |
| G: -4276.08596 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10540.91899 HOMO: -6.63958 LUMO: 1.84221 factor:1 | 1 (-0.46733) | -1 | -1 |
| G: -4276.08596 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10541.05137 HOMO: -6.70761 LUMO: 1.67350 factor:1 | 1 (-0.59971) | -1 | -1 |
| G: -4276.08596 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10541.08190 HOMO: -6.00283 LUMO: 1.64357 factor:1 | 1 (-0.63024) | -1 | -1 |
| G: -4276.08596 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10540.89392 HOMO: -6.48719 LUMO: 1.70343 factor:1 | 1 (-0.44227) | -1 | -1 |
| G: -4276.08596 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10541.16748 HOMO: -6.13345 LUMO: 1.44492 factor:1 | 1 (-0.71582) | -1 | -1 |
| G: -4276.08596 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10541.03093 HOMO: -6.11168 LUMO: 1.70071 factor:1 | 1 (-0.57928) | -1 | -1 |
| G: -4276.08596 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10540.89186 HOMO: -6.09535 LUMO: 1.82316 factor:1 | 1 (-0.44020) | -1 | -1 |
| G: -4276.08596 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10540.75131 HOMO: -6.81101 LUMO: 1.63540 factor:1 | 1 (-0.29965) | -1 | -1 |
| G: -4276.08596 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10541.02217 HOMO: -6.80013 LUMO: 2.12249 factor:1 | 1 (-0.57051) | -1 | -1 |
| G: -4276.08596 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10540.81771 HOMO: -6.48447 LUMO: 1.94561 factor:1 | 1 (-0.36605) | -1 | -1 |
| G: -4276.08596 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10540.72181 HOMO: -6.72393 LUMO: 2.06534 factor:1 | 1 (-0.27015) | -1 | -1 |
| G: -4276.08596 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10540.62241 HOMO: -6.34570 LUMO: 1.98915 factor:1 | 1 (-0.17075) | -1 | -1 |
| G: -4276.08596 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10540.76530 HOMO: -6.31304 LUMO: 1.87759 factor:1 | 1 (-0.31364) | -1 | -1 |
| G: -4276.08596 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10540.85194 HOMO: -6.77564 LUMO: 1.81228 factor:1 | 1 (-0.40028) | -1 | -1 |
| G: -4276.08596 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10540.80873 HOMO: -6.58516 LUMO: 2.34834 factor:1 | 1 (-0.35707) | -1 | -1 |
| G: -4276.08596 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10540.59754 HOMO: -6.68040 LUMO: 2.20412 factor:1 | 1 (-0.14588) | -1 | -1 |
| G: -4276.08596 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10540.93292 HOMO: -6.20964 LUMO: 2.17147 factor:1 | 1 (-0.48126) | -1 | -1 |
| G: -4276.08596 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10540.88097 HOMO: -6.54706 LUMO: 2.03813 factor:1 | 1 (-0.42931) | -1 | -1 |
| G: -4276.08596 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10541.02424 HOMO: -6.54162 LUMO: 2.17419 factor:1 | 1 (-0.57258) | -1 | -1 |
| G: -4276.08596 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10540.85703 HOMO: -6.75659 LUMO: 2.22589 factor:1 | 1 (-0.40537) | -1 | -1 |
| G: -4276.08596 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10540.99678 HOMO: -6.59604 LUMO: 2.59325 factor:1 | 1 (-0.54513) | -1 | -1 |
| G: -4276.08596 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10540.96718 HOMO: -6.11712 LUMO: 2.02181 factor:1 | 1 (-0.51552) | -1 | -1 |
| G: -4276.08596 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10540.84998 HOMO: -6.63141 LUMO: 2.09256 factor:1 | 1 (-0.39832) | -1 | -1 |
| G: -4276.08596 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10540.94040 HOMO: -6.61781 LUMO: 1.86126 factor:1 | 1 (-0.48874) | -1 | -1 |
| G: -4276.08596 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10540.84538 HOMO: -6.63958 LUMO: 1.77146 factor:1 | 1 (-0.39372) | -1 | -1 |
| G: -4276.08596 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10540.63550 HOMO: -6.60420 LUMO: 1.54561 factor:1 | 1 (-0.18384) | -1 | -1 |
| G: -4276.08596 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10540.87169 HOMO: -6.52529 LUMO: 2.05174 factor:1 | 1 (-0.42003) | -1 | -1 |
| G: -4276.08596 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10540.65436 HOMO: -6.80285 LUMO: 2.13609 factor:1 | 1 (-0.20270) | -1 | -1 |
| G: -4276.08596 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10540.78366 HOMO: -6.51168 LUMO: 2.25855 factor:1 | 1 (-0.33201) | -1 | -1 |
| G: -4276.08596 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10540.71920 HOMO: -6.64774 LUMO: 2.46263 factor:1 | 1 (-0.26754) | -1 | -1 |
| G: -4276.08596 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10540.53000 HOMO: -6.40828 LUMO: 1.99732 factor:1 | 1 (-0.07834) | -1 | -1 |
| G: -4276.08596 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10540.91482 HOMO: -5.97562 LUMO: 1.56465 factor:1 | 1 (-0.46317) | -1 | -1 |
| G: -4276.04229 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10541.17962 HOMO: -6.75659 LUMO: 2.23405 factor:1 | 1 (-0.77163) | -1 | -1 |
| G: -4276.04229 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10541.31883 HOMO: -6.68584 LUMO: 2.09528 factor:1 | 1 (-0.91085) | -1 | -1 |
| G: -4276.04229 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10541.07785 HOMO: -6.86543 LUMO: 1.95106 factor:1 | 1 (-0.66986) | -1 | -1 |
| G: -4276.04229 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10541.05439 HOMO: -6.47359 LUMO: 1.82316 factor:1 | 1 (-0.64641) | -1 | -1 |
| G: -4276.04229 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10541.28571 HOMO: -6.87632 LUMO: 2.08439 factor:1 | 1 (-0.87773) | -1 | -1 |
| G: -4276.04229 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10541.01137 HOMO: -6.33753 LUMO: 2.16603 factor:1 | 1 (-0.60339) | -1 | -1 |
| G: -4276.04229 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10541.05447 HOMO: -6.92258 LUMO: 1.72248 factor:1 | 1 (-0.64649) | -1 | -1 |
| G: -4276.04229 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10541.14209 HOMO: -6.62597 LUMO: 2.10344 factor:1 | 1 (-0.73411) | -1 | -1 |
| G: -4276.04229 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10541.21605 HOMO: -6.63141 LUMO: 1.94017 factor:1 | 1 (-0.80807) | -1 | -1 |
| G: -4276.04229 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10540.94843 HOMO: -6.48447 LUMO: 1.91840 factor:1 | 1 (-0.54045) | -1 | -1 |
| G: -4276.04229 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10540.88459 HOMO: -6.41372 LUMO: 1.61364 factor:1 | 1 (-0.47661) | -1 | -1 |
| G: -4276.04229 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10541.09194 HOMO: -6.37291 LUMO: 1.79051 factor:1 | 1 (-0.68396) | -1 | -1 |
| G: -4276.04229 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10541.01839 HOMO: -6.13073 LUMO: 1.77962 factor:1 | 1 (-0.61041) | -1 | -1 |
| G: -4276.04229 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10541.21926 HOMO: -6.13073 LUMO: 1.98915 factor:1 | 1 (-0.81128) | -1 | -1 |
| G: -4276.04229 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10540.97610 HOMO: -6.44094 LUMO: 1.58370 factor:1 | 1 (-0.56812) | -1 | -1 |
| G: -4276.04229 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10540.78287 HOMO: -6.87087 LUMO: -0.82995 factor:1 | 1 (-0.37489) | -1 | -1 |
| G: -4276.04229 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10540.74739 HOMO: -6.67223 LUMO: 1.08029 factor:1 | 1 (-0.33941) | -1 | -1 |
| G: -4276.04229 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10540.63762 HOMO: -6.82462 LUMO: 0.91702 factor:1 | 1 (-0.22964) | -1 | -1 |
| G: -4276.04229 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10541.13523 HOMO: -6.65863 LUMO: 1.52656 factor:1 | 1 (-0.72725) | -1 | -1 |
| G: -4276.04229 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10540.98005 HOMO: -6.78924 LUMO: 0.86260 factor:1 | 1 (-0.57206) | -1 | -1 |
| G: -4276.04229 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10541.31146 HOMO: -6.68584 LUMO: 0.94424 factor:1 | 1 (-0.90347) | -1 | -1 |
| G: -4276.04229 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10540.92524 HOMO: -6.58788 LUMO: 1.00138 factor:1 | 1 (-0.51726) | -1 | -1 |
| G: -4276.04229 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10541.10653 HOMO: -6.79740 LUMO: 0.91430 factor:1 | 1 (-0.69854) | -1 | -1 |
| G: -4276.04229 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10541.26082 HOMO: -6.67223 LUMO: 0.80274 factor:1 | 1 (-0.85283) | -1 | -1 |
| G: -4276.04229 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10541.16179 HOMO: -6.95251 LUMO: 0.90614 factor:1 | 1 (-0.75381) | -1 | -1 |
| G: -4276.04229 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10541.10963 HOMO: -7.19469 LUMO: 1.34152 factor:1 | 1 (-0.70165) | -1 | -1 |
| G: -4276.04229 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10541.10182 HOMO: -6.59332 LUMO: -0.76464 factor:1 | 1 (-0.69384) | -1 | -1 |
| G: -4276.04229 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10541.24307 HOMO: -6.77564 LUMO: -0.90886 factor:1 | 1 (-0.83509) | -1 | -1 |
| G: -4276.04229 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10541.07436 HOMO: -6.57971 LUMO: -0.41633 factor:1 | 1 (-0.66638) | -1 | -1 |
| G: -4276.04229 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10540.97382 HOMO: -6.68856 LUMO: -0.58232 factor:1 | 1 (-0.56583) | -1 | -1 |
| G: -4276.04229 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10540.93950 HOMO: -6.87087 LUMO: -0.71022 factor:1 | 1 (-0.53152) | -1 | -1 |
| G: -4276.04229 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10541.08462 HOMO: -6.67767 LUMO: -0.74559 factor:1 | 1 (-0.67664) | -1 | -1 |
| G: -4276.04229 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10541.01496 HOMO: -6.68040 LUMO: -0.65307 factor:1 | 1 (-0.60698) | -1 | -1 |
| G: -4276.04229 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10541.04239 HOMO: -6.32937 LUMO: 0.80274 factor:1 | 1 (-0.63441) | -1 | -1 |
| G: -4276.04229 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10540.88383 HOMO: -6.29671 LUMO: 0.82723 factor:1 | 1 (-0.47585) | -1 | -1 |
| G: -4276.04229 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10540.72451 HOMO: -6.67767 LUMO: 0.59321 factor:1 | 1 (-0.31652) | -1 | -1 |
| G: -4276.04229 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10540.84464 HOMO: -6.77836 LUMO: 0.50341 factor:1 | 1 (-0.43666) | -1 | -1 |
| G: -4276.04229 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10541.08914 HOMO: -6.61781 LUMO: 0.42450 factor:1 | 1 (-0.68116) | -1 | -1 |
| G: -4276.04229 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10540.86791 HOMO: -6.83278 LUMO: 0.39457 factor:1 | 1 (-0.45993) | -1 | -1 |
| G: -4276.04229 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10540.97390 HOMO: -6.56883 LUMO: 0.64219 factor:1 | 1 (-0.56592) | -1 | -1 |
| G: -4276.04229 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10540.74579 HOMO: -6.71577 LUMO: 0.40001 factor:1 | 1 (-0.33780) | -1 | -1 |
| G: -4276.04229 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10540.71057 HOMO: -6.86543 LUMO: -0.74287 factor:1 | 1 (-0.30259) | -1 | -1 |
| G: -4276.04229 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10540.54782 HOMO: -6.68584 LUMO: -0.69389 factor:1 | 1 (-0.13984) | -1 | -1 |
| G: -4276.04229 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10541.04982 HOMO: -6.61237 LUMO: -0.48980 factor:1 | 1 (-0.64183) | -1 | -1 |
| G: -4276.04229 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10541.00078 HOMO: -6.80285 LUMO: -0.58232 factor:1 | 1 (-0.59280) | -1 | -1 |
| G: -4276.04229 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10541.29954 HOMO: -6.88992 LUMO: -0.70205 factor:1 | 1 (-0.89155) | -1 | -1 |
| G: -4276.04229 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10541.10215 HOMO: -6.95251 LUMO: -0.71838 factor:1 | 1 (-0.69416) | -1 | -1 |
| G: -4276.04229 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10540.86709 HOMO: -7.52123 LUMO: 0.27211 factor:1 | 1 (-0.45911) | -1 | -1 |
| G: -4276.04229 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10540.83743 HOMO: -6.76747 LUMO: -0.74015 factor:1 | 1 (-0.42945) | -1 | -1 |
| G: -4276.04229 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10541.27458 HOMO: -6.55250 LUMO: -0.49797 factor:1 | 1 (-0.86660) | -1 | -1 |
| G: -4276.04229 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10541.14775 HOMO: -6.50896 LUMO: -0.46804 factor:1 | 1 (-0.73977) | -1 | -1 |
| G: -4276.04229 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10540.86576 HOMO: -7.45320 LUMO: 0.08436 factor:1 | 1 (-0.45778) | -1 | -1 |
| G: -4276.04229 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10540.78579 HOMO: -6.82462 LUMO: -0.70477 factor:1 | 1 (-0.37780) | -1 | -1 |
| G: -4276.04229 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10541.14873 HOMO: -6.57155 LUMO: -0.43538 factor:1 | 1 (-0.74075) | -1 | -1 |
| G: -4276.04229 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10540.82222 HOMO: -6.72665 LUMO: -0.55239 factor:1 | 1 (-0.41424) | -1 | -1 |
| G: -4276.04229 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10541.09251 HOMO: -7.05319 LUMO: -1.08573 factor:1 | 1 (-0.68453) | -1 | -1 |
| G: -4276.04229 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10541.06383 HOMO: -6.56067 LUMO: -0.45715 factor:1 | 1 (-0.65585) | -1 | -1 |
| G: -4276.04229 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10541.02122 HOMO: -6.76475 LUMO: -0.53879 factor:1 | 1 (-0.61324) | -1 | -1 |
| G: -4276.04229 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10541.22754 HOMO: -6.67223 LUMO: -0.45987 factor:1 | 1 (-0.81955) | -1 | -1 |
| G: -4276.04229 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10540.75011 HOMO: -6.44094 LUMO: -0.72110 factor:1 | 1 (-0.34213) | -1 | -1 |
| G: -4276.04229 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10540.69800 HOMO: -6.66951 LUMO: -0.67756 factor:1 | 1 (-0.29002) | -1 | -1 |
| G: -4276.04229 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10540.91899 HOMO: -6.69400 LUMO: -0.62858 factor:1 | 1 (-0.51100) | -1 | -1 |
| G: -4276.04229 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10541.05137 HOMO: -6.51985 LUMO: -0.37007 factor:1 | 1 (-0.64339) | -1 | -1 |
| G: -4276.04229 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10541.08190 HOMO: -5.98378 LUMO: 0.78641 factor:1 | 1 (-0.67392) | -1 | -1 |
| G: -4276.04229 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10540.89392 HOMO: -6.11440 LUMO: 0.71294 factor:1 | 1 (-0.48594) | -1 | -1 |
| G: -4276.04229 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10541.16748 HOMO: -6.45182 LUMO: 0.63947 factor:1 | 1 (-0.75950) | -1 | -1 |
| G: -4276.04229 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10541.03093 HOMO: -6.78924 LUMO: 0.37007 factor:1 | 1 (-0.62295) | -1 | -1 |
| G: -4276.04229 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10540.89186 HOMO: -6.63686 LUMO: 0.54423 factor:1 | 1 (-0.48387) | -1 | -1 |
| G: -4276.04229 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10540.75131 HOMO: -6.66679 LUMO: 0.48708 factor:1 | 1 (-0.34333) | -1 | -1 |
| G: -4276.04229 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10541.02217 HOMO: -6.81917 LUMO: 0.31021 factor:1 | 1 (-0.61419) | -1 | -1 |
| G: -4276.04229 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10540.81771 HOMO: -6.28583 LUMO: 0.44899 factor:1 | 1 (-0.40972) | -1 | -1 |
| G: -4276.04229 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10540.72181 HOMO: -6.61237 LUMO: 0.49525 factor:1 | 1 (-0.31383) | -1 | -1 |
| G: -4276.04229 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10540.62241 HOMO: -7.08857 LUMO: 0.38368 factor:1 | 1 (-0.21443) | -1 | -1 |
| G: -4276.04229 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10540.76530 HOMO: -6.53890 LUMO: -0.68845 factor:1 | 1 (-0.35731) | -1 | -1 |
| G: -4276.04229 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10540.85194 HOMO: -6.56611 LUMO: -0.66396 factor:1 | 1 (-0.44395) | -1 | -1 |
| G: -4276.04229 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10540.80873 HOMO: -6.04909 LUMO: -0.59865 factor:1 | 1 (-0.40074) | -1 | -1 |
| G: -4276.04229 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10540.59754 HOMO: -6.74842 LUMO: -0.77825 factor:1 | 1 (-0.18955) | -1 | -1 |
| G: -4276.04229 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10540.93292 HOMO: -6.82462 LUMO: -0.61498 factor:1 | 1 (-0.52493) | -1 | -1 |
| G: -4276.04229 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10540.88097 HOMO: -7.40694 LUMO: 0.32926 factor:1 | 1 (-0.47299) | -1 | -1 |
| G: -4276.04229 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10541.02424 HOMO: -6.80557 LUMO: -0.57416 factor:1 | 1 (-0.61626) | -1 | -1 |
| G: -4276.04229 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10540.85703 HOMO: -6.76747 LUMO: -0.67484 factor:1 | 1 (-0.44904) | -1 | -1 |
| G: -4276.04229 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10540.99678 HOMO: -7.23279 LUMO: 0.48980 factor:1 | 1 (-0.58880) | -1 | -1 |
| G: -4276.04229 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10540.96718 HOMO: -6.62869 LUMO: -0.24762 factor:1 | 1 (-0.55919) | -1 | -1 |
| G: -4276.04229 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10540.84998 HOMO: -6.65863 LUMO: -0.28028 factor:1 | 1 (-0.44199) | -1 | -1 |
| G: -4276.04229 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10540.94040 HOMO: -6.50352 LUMO: -0.44899 factor:1 | 1 (-0.53242) | -1 | -1 |
| G: -4276.04229 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10540.84538 HOMO: -6.62053 LUMO: -0.88437 factor:1 | 1 (-0.43740) | -1 | -1 |
| G: -4276.04229 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10540.63550 HOMO: -6.73754 LUMO: -0.77825 factor:1 | 1 (-0.22751) | -1 | -1 |
| G: -4276.04229 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10540.87169 HOMO: -7.24639 LUMO: 0.35647 factor:1 | 1 (-0.46371) | -1 | -1 |
| G: -4276.04229 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10540.65436 HOMO: -6.46270 LUMO: -0.48164 factor:1 | 1 (-0.24637) | -1 | -1 |
| G: -4276.04229 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10540.78366 HOMO: -6.14161 LUMO: -0.66396 factor:1 | 1 (-0.37568) | -1 | -1 |
| G: -4276.04229 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10540.71920 HOMO: -6.63414 LUMO: 1.51295 factor:1 | 1 (-0.31122) | -1 | -1 |
| G: -4276.04229 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10540.53000 HOMO: -6.52529 LUMO: 1.65989 factor:1 | 1 (-0.12202) | -1 | -1 |
| G: -4276.04229 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10540.91482 HOMO: -6.63686 LUMO: 1.64629 factor:1 | 1 (-0.50684) | -1 | -1 |
| G: -5717.87902 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.16644 HOMO: -6.49808 LUMO: 1.60003 factor:1 | -1 (1.07828) | -1 | -1 |
| G: -5717.87902 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.55948 HOMO: -6.85183 LUMO: 1.96194 factor:1 | -1 (0.68524) | -1 | -1 |
| G: -5717.87902 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.40174 HOMO: -6.90081 LUMO: 1.82316 factor:1 | -1 (1.84297) | -1 | -1 |
| G: -5717.87902 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.48163 HOMO: -6.20147 LUMO: 1.95106 factor:1 | -1 (1.76308) | -1 | -1 |
| G: -5717.87902 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.37668 HOMO: -7.05047 LUMO: 1.94289 factor:1 | -1 (1.86803) | -1 | -1 |
| G: -5717.87902 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.45962 HOMO: -6.11440 LUMO: 1.83949 factor:1 | -1 (1.78509) | -1 | -1 |
| G: -5717.87902 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.50193 HOMO: -6.65046 LUMO: 1.59187 factor:1 | -1 (1.74278) | -1 | -1 |
| G: -5717.87902 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.43216 HOMO: -6.81917 LUMO: 2.41365 factor:1 | -1 (1.81255) | -1 | -1 |
| G: -5717.87902 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.47709 HOMO: -6.40284 LUMO: 2.48984 factor:1 | -1 (1.76762) | -1 | -1 |
| G: -5717.87902 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.06097 HOMO: -7.04775 LUMO: 2.31025 factor:1 | -1 (1.18375) | -1 | -1 |
| G: -5717.87902 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.17759 HOMO: -6.64774 LUMO: 2.20140 factor:1 | -1 (1.06712) | -1 | -1 |
| G: -5717.87902 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.19719 HOMO: -6.72393 LUMO: 2.28304 factor:1 | -1 (1.04753) | -1 | -1 |
| G: -5717.87902 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.54593 HOMO: -6.35114 LUMO: 1.84765 factor:1 | -1 (0.69879) | -1 | -1 |
| G: -5717.87902 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.46677 HOMO: -6.41100 LUMO: 1.74697 factor:1 | -1 (0.77795) | -1 | -1 |
| G: -5717.87902 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.26871 HOMO: -6.34297 LUMO: 1.55921 factor:1 | -1 (1.97601) | -1 | -1 |
| G: -5717.87902 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.40876 HOMO: -6.31848 LUMO: 1.67622 factor:1 | -1 (1.83595) | -1 | -1 |
| G: -5717.87902 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.11442 HOMO: -6.50896 LUMO: 2.02725 factor:1 | -1 (2.13030) | -1 | -1 |
| G: -5717.87902 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.38253 HOMO: -6.28583 LUMO: 2.00548 factor:1 | -1 (1.86218) | -1 | -1 |
| G: -5717.87902 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.39693 HOMO: -6.67495 LUMO: 1.92384 factor:1 | -1 (1.84779) | -1 | -1 |
| G: -5717.87902 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.17667 HOMO: -6.17154 LUMO: 2.39732 factor:1 | -1 (1.06805) | -1 | -1 |
| G: -5717.87902 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.87269 HOMO: -6.84911 LUMO: 2.24766 factor:1 | -1 (1.37203) | -1 | -1 |
| G: -5717.87902 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.06785 HOMO: -6.77564 LUMO: 2.38372 factor:1 | -1 (1.17687) | -1 | -1 |
| G: -5717.87902 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.19310 HOMO: -6.18243 LUMO: 2.40821 factor:1 | -1 (1.05161) | -1 | -1 |
| G: -5717.87902 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.38095 HOMO: -6.40828 LUMO: 2.22589 factor:1 | -1 (1.86376) | -1 | -1 |
| G: -5717.87902 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.44988 HOMO: -6.74570 LUMO: 1.88303 factor:1 | -1 (1.79484) | -1 | -1 |
| G: -5717.87902 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.14434 HOMO: -6.29944 LUMO: 2.05174 factor:1 | -1 (1.10037) | -1 | -1 |
| G: -5717.87902 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.06932 HOMO: -7.00693 LUMO: 2.16331 factor:1 | -1 (1.17540) | -1 | -1 |
| G: -5717.87902 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.14551 HOMO: -6.89537 LUMO: 2.19596 factor:1 | -1 (1.09920) | -1 | -1 |
| G: -5717.87902 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.44173 HOMO: -6.72665 LUMO: 2.03813 factor:1 | -1 (0.80298) | -1 | -1 |
| G: -5717.87902 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.37505 HOMO: -6.69944 LUMO: 2.36467 factor:1 | -1 (1.86967) | -1 | -1 |
| G: -5717.87902 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.12941 HOMO: -6.92802 LUMO: 1.72792 factor:1 | -1 (2.11530) | -1 | -1 |
| G: -5717.87902 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.35845 HOMO: -6.12256 LUMO: 1.85310 factor:1 | -1 (1.88627) | -1 | -1 |
| G: -5717.87902 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.33594 HOMO: -6.70489 LUMO: 2.20956 factor:1 | -1 (1.90877) | -1 | -1 |
| G: -5717.87902 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.39290 HOMO: -6.94707 LUMO: 1.81500 factor:1 | -1 (1.85182) | -1 | -1 |
| G: -5717.87902 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.45965 HOMO: -6.39468 LUMO: 1.79051 factor:1 | -1 (1.78507) | -1 | -1 |
| G: -5717.87902 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.32109 HOMO: -6.69128 LUMO: 2.03813 factor:1 | -1 (1.92363) | -1 | -1 |
| G: -5717.87902 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.38065 HOMO: -6.55250 LUMO: 2.00548 factor:1 | -1 (1.86406) | -1 | -1 |
| G: -5717.87902 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.42474 HOMO: -6.24773 LUMO: 2.09256 factor:1 | -1 (1.81998) | -1 | -1 |
| G: -5717.87902 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.07931 HOMO: -6.85727 LUMO: 1.70071 factor:1 | -1 (1.16541) | -1 | -1 |
| G: -5717.87902 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.87049 HOMO: -6.71305 LUMO: 1.72520 factor:1 | -1 (1.37423) | -1 | -1 |
| G: -5717.87902 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.18203 HOMO: -6.81101 LUMO: 2.15514 factor:1 | -1 (1.06269) | -1 | -1 |
| G: -5717.87902 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.18187 HOMO: -6.93618 LUMO: 1.75513 factor:1 | -1 (2.06284) | -1 | -1 |
| G: -5717.87902 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.32876 HOMO: -6.63686 LUMO: 2.09800 factor:1 | -1 (1.91595) | -1 | -1 |
| G: -5717.87902 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.05128 HOMO: -6.98244 LUMO: 1.72520 factor:1 | -1 (1.19344) | -1 | -1 |
| G: -5717.87902 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.06167 HOMO: -6.37019 LUMO: 2.35923 factor:1 | -1 (1.18304) | -1 | -1 |
| G: -5717.87902 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.10853 HOMO: -6.55794 LUMO: 2.12521 factor:1 | -1 (1.13618) | -1 | -1 |
| G: -5717.87902 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.10497 HOMO: -6.45998 LUMO: 1.93201 factor:1 | -1 (1.13975) | -1 | -1 |
| G: -5717.87902 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.23483 HOMO: -6.71033 LUMO: 1.58370 factor:1 | -1 (2.00989) | -1 | -1 |
| G: -5717.87902 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.06778 HOMO: -6.67223 LUMO: 1.52928 factor:1 | -1 (2.17694) | -1 | -1 |
| G: -5717.87902 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.17567 HOMO: -6.72121 LUMO: 1.33608 factor:1 | -1 (2.06904) | -1 | -1 |
| G: -5717.87902 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11979.99120 HOMO: -6.89264 LUMO: 2.08983 factor:1 | -1 (2.25351) | -1 | -1 |
| G: -5717.87902 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.15401 HOMO: -6.31032 LUMO: 2.24766 factor:1 | -1 (2.09071) | -1 | -1 |
| G: -5717.87902 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.12820 HOMO: -6.79740 LUMO: 2.09528 factor:1 | -1 (1.11651) | -1 | -1 |
| G: -5717.87902 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.10271 HOMO: -6.78108 LUMO: 2.15786 factor:1 | -1 (1.14201) | -1 | -1 |
| G: -5717.87902 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.34707 HOMO: -6.50896 LUMO: 2.15786 factor:1 | -1 (1.89764) | -1 | -1 |
| G: -5717.87902 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.26558 HOMO: -6.56067 LUMO: 2.24494 factor:1 | -1 (1.97914) | -1 | -1 |
| G: -5717.87902 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.40797 HOMO: -6.72938 LUMO: 2.24494 factor:1 | -1 (1.83674) | -1 | -1 |
| G: -5717.87902 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.08408 HOMO: -6.40556 LUMO: 1.58642 factor:1 | -1 (2.16064) | -1 | -1 |
| G: -5717.87902 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.12753 HOMO: -6.63141 LUMO: 1.66262 factor:1 | -1 (2.11718) | -1 | -1 |
| G: -5717.87902 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.07131 HOMO: -6.97156 LUMO: 2.23678 factor:1 | -1 (2.17340) | -1 | -1 |
| G: -5717.87902 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.21692 HOMO: -6.86271 LUMO: 1.91296 factor:1 | -1 (2.02779) | -1 | -1 |
| G: -5717.87902 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.15626 HOMO: -6.50624 LUMO: 1.89119 factor:1 | -1 (1.08846) | -1 | -1 |
| G: -5717.87902 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.27581 HOMO: -6.70761 LUMO: 1.56193 factor:1 | -1 (1.96891) | -1 | -1 |
| G: -5717.87902 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.23864 HOMO: -6.60420 LUMO: 1.79595 factor:1 | -1 (2.00608) | -1 | -1 |
| G: -5717.87902 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.03199 HOMO: -6.85727 LUMO: 2.26943 factor:1 | -1 (2.21272) | -1 | -1 |
| G: -5717.87902 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.34248 HOMO: -6.23413 LUMO: 1.91024 factor:1 | -1 (1.90224) | -1 | -1 |
| G: -5717.87902 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.34841 HOMO: -6.84366 LUMO: 2.01364 factor:1 | -1 (1.89631) | -1 | -1 |
| G: -5717.87902 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.97770 HOMO: -6.63414 LUMO: 2.54971 factor:1 | -1 (1.26702) | -1 | -1 |
| G: -5717.87902 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.16557 HOMO: -6.52257 LUMO: 2.42998 factor:1 | -1 (1.07915) | -1 | -1 |
| G: -5717.87902 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.92314 HOMO: -6.61509 LUMO: 2.31297 factor:1 | -1 (1.32158) | -1 | -1 |
| G: -5717.87902 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.81595 HOMO: -6.45998 LUMO: 2.23405 factor:1 | -1 (1.42876) | -1 | -1 |
| G: -5717.87902 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.97645 HOMO: -6.86271 LUMO: 2.22317 factor:1 | -1 (1.26827) | -1 | -1 |
| G: -5717.87902 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.09714 HOMO: -6.84366 LUMO: 2.11432 factor:1 | -1 (2.14758) | -1 | -1 |
| G: -5717.87902 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.03711 HOMO: -6.85999 LUMO: 2.44902 factor:1 | -1 (2.20761) | -1 | -1 |
| G: -5717.87902 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.18274 HOMO: -6.73482 LUMO: 1.93745 factor:1 | -1 (2.06197) | -1 | -1 |
| G: -5717.87902 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11979.94688 HOMO: -6.91441 LUMO: 2.32385 factor:1 | -1 (2.29784) | -1 | -1 |
| G: -5717.87902 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.16873 HOMO: -6.16066 LUMO: 2.26399 factor:1 | -1 (2.07598) | -1 | -1 |
| G: -5717.87902 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.29230 HOMO: -6.71305 LUMO: 2.38644 factor:1 | -1 (1.95242) | -1 | -1 |
| G: -5717.87902 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.06818 HOMO: -7.08312 LUMO: 2.01636 factor:1 | -1 (2.17653) | 1 | 1 |
| G: -5717.87902 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.32381 HOMO: -6.15249 LUMO: 1.90752 factor:1 | -1 (1.92091) | -1 | -1 |
| G: -5717.87902 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.32392 HOMO: -6.83006 LUMO: 2.25855 factor:1 | -1 (1.92080) | -1 | -1 |
| G: -5717.87902 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.33246 HOMO: -6.77836 LUMO: 2.24766 factor:1 | -1 (1.91225) | -1 | -1 |
| G: -5717.87902 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11979.99673 HOMO: -6.66951 LUMO: 2.35923 factor:1 | -1 (2.24799) | -1 | -1 |
| G: -5717.87902 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.83220 HOMO: -6.68312 LUMO: 2.30208 factor:1 | -1 (1.41252) | -1 | -1 |
| G: -5717.87902 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.93138 HOMO: -6.49808 LUMO: 2.49801 factor:1 | -1 (1.31333) | -1 | -1 |
| G: -5717.87902 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.96311 HOMO: -6.62325 LUMO: 1.89935 factor:1 | -1 (1.28160) | -1 | -1 |
| G: -5717.87902 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.21961 HOMO: -6.80829 LUMO: 1.91296 factor:1 | -1 (1.02511) | -1 | -1 |
| G: -5717.87902 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.61309 HOMO: -6.64230 LUMO: 2.13065 factor:1 | -1 (1.63162) | -1 | -1 |
| G: -5717.87902 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.72425 HOMO: -6.40556 LUMO: 1.83949 factor:1 | -1 (1.52046) | -1 | -1 |
| G: -5717.87902 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.05046 HOMO: -6.48175 LUMO: 1.72248 factor:1 | -1 (1.19425) | -1 | -1 |
| G: -5717.87902 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.10687 HOMO: -6.61781 LUMO: 2.11432 factor:1 | -1 (1.13784) | -1 | -1 |
| G: -5717.87902 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.94725 HOMO: -6.34570 LUMO: 2.22317 factor:1 | -1 (1.29747) | -1 | -1 |
| G: -5717.87902 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.06056 HOMO: -7.00149 LUMO: 1.80139 factor:1 | -1 (1.18416) | -1 | -1 |
| G: -5717.87902 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.94787 HOMO: -6.66951 LUMO: 2.13065 factor:1 | -1 (1.29684) | -1 | -1 |
| G: -5717.87902 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.12141 HOMO: -6.54434 LUMO: 2.20140 factor:1 | -1 (2.12330) | -1 | -1 |
| G: -5717.87902 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.12152 HOMO: -6.67767 LUMO: 2.02997 factor:1 | -1 (2.12320) | -1 | -1 |
| G: -5717.87902 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11979.94160 HOMO: -6.49536 LUMO: 2.42998 factor:1 | -1 (2.30312) | -1 | -1 |
| G: -5717.87902 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.17771 HOMO: -6.70761 LUMO: 2.71025 factor:1 | -1 (2.06700) | -1 | -1 |
| G: -5717.87902 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.16944 HOMO: -6.62869 LUMO: 2.11160 factor:1 | -1 (2.07528) | -1 | -1 |
| G: -5717.87902 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.01482 HOMO: -6.61781 LUMO: 2.24494 factor:1 | -1 (2.22989) | -1 | -1 |
| G: -5717.87902 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.11053 HOMO: -6.66135 LUMO: 2.20956 factor:1 | -1 (2.13419) | -1 | -1 |
| G: -5717.87902 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.15406 HOMO: -6.95523 LUMO: 2.03813 factor:1 | -1 (2.09065) | -1 | -1 |
| G: -5717.87902 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.37303 HOMO: -7.11578 LUMO: 2.41365 factor:1 | -1 (1.87168) | 1 | 1 |
| G: -5717.87902 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.44563 HOMO: -6.99061 LUMO: 2.13881 factor:1 | -1 (1.79908) | -1 | -1 |
| G: -5717.87902 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.22470 HOMO: -6.43277 LUMO: 2.01364 factor:1 | -1 (2.02001) | -1 | -1 |
| G: -5717.87902 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.27466 HOMO: -6.79196 LUMO: 2.04358 factor:1 | -1 (1.97005) | -1 | -1 |
| G: -5717.87902 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.06252 HOMO: -7.08584 LUMO: 1.99732 factor:1 | -1 (2.18219) | 1 | 1 |
| G: -5717.87902 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.06952 HOMO: -6.46815 LUMO: 2.29936 factor:1 | -1 (2.17520) | -1 | -1 |
| G: -5717.87902 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.27730 HOMO: -6.78108 LUMO: 1.93745 factor:1 | -1 (1.96741) | -1 | -1 |
| G: -5717.87902 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.12530 HOMO: -6.43277 LUMO: 1.80956 factor:1 | -1 (2.11941) | -1 | -1 |
| G: -5717.87902 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.28242 HOMO: -6.71577 LUMO: -0.81090 factor:1 | -1 (1.96229) | -1 | -1 |
| G: -5717.87902 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11979.95452 HOMO: -7.14027 LUMO: -0.68028 factor:1 | -1 (2.29019) | -1 | -1 |
| G: -5717.87902 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.92567 HOMO: -7.03414 LUMO: -0.69661 factor:1 | -1 (1.31904) | -1 | -1 |
| G: -5717.87902 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.84559 HOMO: -6.64502 LUMO: -0.47348 factor:1 | -1 (1.39913) | -1 | -1 |
| G: -5717.87902 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.37127 HOMO: -6.60692 LUMO: 2.12793 factor:1 | -1 (1.87345) | -1 | -1 |
| G: -5717.87902 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.80148 HOMO: -6.66407 LUMO: 1.94561 factor:1 | -1 (1.44324) | -1 | -1 |
| G: -5717.87902 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.93666 HOMO: -7.10217 LUMO: 1.92384 factor:1 | -1 (1.30805) | 1 | 1 |
| G: -5717.87902 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.74569 HOMO: -6.84094 LUMO: 1.66534 factor:1 | -1 (1.49902) | -1 | -1 |
| G: -5717.87902 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.10067 HOMO: -6.93618 LUMO: 2.13065 factor:1 | -1 (1.14405) | -1 | -1 |
| G: -5717.87902 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.09189 HOMO: -6.60692 LUMO: 2.20684 factor:1 | -1 (2.15283) | -1 | -1 |
| G: -5717.87902 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11979.83479 HOMO: -6.85727 LUMO: 2.19324 factor:1 | -1 (2.40992) | -1 | -1 |
| G: -5717.87902 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.07235 HOMO: -6.31032 LUMO: 1.76330 factor:1 | -1 (2.17237) | -1 | -1 |
| G: -5717.87902 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.26324 HOMO: -6.43821 LUMO: 2.10072 factor:1 | -1 (1.98148) | -1 | -1 |
| G: -5717.87902 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.29662 HOMO: -6.42189 LUMO: 2.19596 factor:1 | -1 (1.94809) | -1 | -1 |
| G: -5717.87902 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.02228 HOMO: -6.40556 LUMO: 2.02181 factor:1 | -1 (2.22244) | -1 | -1 |
| G: -5717.87902 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.07678 HOMO: -6.41372 LUMO: 2.26671 factor:1 | -1 (2.16793) | -1 | -1 |
| G: -5717.87902 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.21232 HOMO: -6.60692 LUMO: 2.09800 factor:1 | -1 (2.03239) | -1 | -1 |
| G: -5717.87902 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.24008 HOMO: -6.75931 LUMO: 1.76602 factor:1 | -1 (2.00464) | -1 | -1 |
| G: -5717.87902 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.15779 HOMO: -6.39195 LUMO: 1.84221 factor:1 | -1 (2.08692) | -1 | -1 |
| G: -5717.87902 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.59576 HOMO: -6.74570 LUMO: 2.04085 factor:1 | -1 (1.64896) | -1 | -1 |
| G: -5717.87902 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.63203 HOMO: -6.77019 LUMO: 2.16875 factor:1 | -1 (1.61268) | -1 | -1 |
| G: -5717.87902 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11979.87771 HOMO: -6.15522 LUMO: 1.81772 factor:1 | -1 (2.36701) | -1 | -1 |
| G: -5717.87902 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11979.76698 HOMO: -6.48175 LUMO: 2.02453 factor:1 | -1 (2.47773) | -1 | -1 |
| G: -5717.87902 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11979.79308 HOMO: -6.57427 LUMO: 1.77962 factor:1 | -1 (2.45164) | -1 | -1 |
| G: -5717.87902 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.32316 HOMO: -6.57699 LUMO: 2.42998 factor:1 | -1 (1.92156) | -1 | -1 |
| G: -5717.87902 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.13616 HOMO: -6.35386 LUMO: 2.25310 factor:1 | -1 (2.10856) | -1 | -1 |
| G: -5717.87902 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.56362 HOMO: -6.80013 LUMO: 2.11160 factor:1 | -1 (1.68109) | -1 | -1 |
| G: -5717.87902 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.35080 HOMO: -6.24229 LUMO: 2.05718 factor:1 | -1 (1.89391) | -1 | -1 |
| G: -5717.87902 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.71799 HOMO: -6.42733 LUMO: 1.76874 factor:1 | -1 (1.52672) | -1 | -1 |
| G: -5717.87902 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.56926 HOMO: -6.56883 LUMO: 2.36195 factor:1 | -1 (1.67546) | -1 | -1 |
| G: -5717.87902 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.62542 HOMO: -6.72665 LUMO: 2.28848 factor:1 | -1 (1.61930) | -1 | -1 |
| G: -5717.87902 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.87593 HOMO: -6.39195 LUMO: 1.79051 factor:1 | -1 (1.36879) | -1 | -1 |
| G: -5717.87902 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.60283 HOMO: -6.70761 LUMO: 0.15510 factor:1 | -1 (1.64188) | -1 | -1 |
| G: -5717.87902 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.92858 HOMO: -6.44366 LUMO: -0.16871 factor:1 | -1 (1.31613) | -1 | -1 |
| G: -5717.87902 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.69971 HOMO: -6.68584 LUMO: 1.69527 factor:1 | -1 (1.54501) | -1 | -1 |
| G: -5717.87902 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.28453 HOMO: -6.26950 LUMO: 1.61636 factor:1 | -1 (0.96018) | -1 | -1 |
| G: -5717.87902 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.35683 HOMO: -6.47631 LUMO: 1.98915 factor:1 | -1 (0.88788) | -1 | -1 |
| G: -5717.87902 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.48791 HOMO: -6.58243 LUMO: 1.97283 factor:1 | -1 (0.75680) | -1 | -1 |
| G: -5717.87902 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.26780 HOMO: -6.51713 LUMO: 1.97283 factor:1 | -1 (0.97692) | -1 | -1 |
| G: -5717.87902 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.08396 HOMO: -6.65046 LUMO: 1.69255 factor:1 | -1 (1.16076) | -1 | -1 |
| G: -5717.87902 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.86955 HOMO: -6.26406 LUMO: 2.21773 factor:1 | -1 (0.37516) | -1 | -1 |
| G: -5717.87902 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.76193 HOMO: -6.88992 LUMO: 2.28304 factor:1 | -1 (0.48278) | -1 | -1 |
| G: -5717.87902 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.80563 HOMO: -6.67767 LUMO: 2.34834 factor:1 | -1 (0.43908) | -1 | -1 |
| G: -5717.87902 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.57523 HOMO: -6.52801 LUMO: 2.10344 factor:1 | -1 (0.66948) | -1 | -1 |
| G: -5717.87902 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.08512 HOMO: -6.52801 LUMO: 2.24222 factor:1 | -1 (0.15959) | -1 | -1 |
| G: -5717.87902 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.57212 HOMO: -6.17154 LUMO: 1.89663 factor:1 | 1 (-0.32741) | -1 | -1 |
| G: -5717.87902 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.59425 HOMO: -6.42733 LUMO: 2.15514 factor:1 | 1 (-0.34953) | -1 | -1 |
| G: -5717.87902 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.52029 HOMO: -6.36474 LUMO: 2.01364 factor:1 | -1 (0.72442) | -1 | -1 |
| G: -5717.87902 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.24735 HOMO: -6.82189 LUMO: 1.86942 factor:1 | 1 (-0.00264) | -1 | -1 |
| G: -5717.87902 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.54334 HOMO: -6.60148 LUMO: 2.00548 factor:1 | -1 (0.70137) | -1 | -1 |
| G: -5717.87902 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.34265 HOMO: -6.67767 LUMO: 2.15786 factor:1 | 1 (-0.09793) | -1 | -1 |
| G: -5717.87902 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11983.03869 HOMO: -6.79196 LUMO: 2.06534 factor:1 | 1 (-0.79397) | -1 | -1 |
| G: -5717.87902 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.38360 HOMO: -6.70216 LUMO: 1.83405 factor:1 | 1 (-0.13889) | -1 | -1 |
| G: -5717.87902 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.09260 HOMO: -6.58788 LUMO: 1.79051 factor:1 | -1 (0.15211) | -1 | -1 |
| G: -5717.87902 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.85608 HOMO: -6.34842 LUMO: 1.80139 factor:1 | -1 (0.38863) | -1 | -1 |
| G: -5717.87902 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.88082 HOMO: -6.48175 LUMO: 1.95922 factor:1 | -1 (0.36390) | -1 | -1 |
| G: -5717.87902 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.56136 HOMO: -6.71033 LUMO: 2.02997 factor:1 | -1 (0.68336) | -1 | -1 |
| G: -5717.87902 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.69792 HOMO: -6.89264 LUMO: 2.42726 factor:1 | 1 (-0.45321) | -1 | -1 |
| G: -5717.87902 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.72524 HOMO: -6.74570 LUMO: 2.20684 factor:1 | 1 (-0.48053) | -1 | -1 |
| G: -5717.87902 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.79396 HOMO: -6.30216 LUMO: 2.15242 factor:1 | -1 (0.45076) | -1 | -1 |
| G: -5717.87902 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.70152 HOMO: -6.94979 LUMO: 2.43814 factor:1 | -1 (0.54319) | -1 | -1 |
| G: -5717.87902 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.75580 HOMO: -6.97972 LUMO: 2.11432 factor:1 | 1 (-0.51108) | -1 | -1 |
| G: -5717.87902 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.53906 HOMO: -6.17154 LUMO: 1.98099 factor:1 | 1 (-0.29435) | -1 | -1 |
| G: -5717.87902 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.10088 HOMO: -6.74026 LUMO: 2.21501 factor:1 | -1 (1.14383) | -1 | -1 |
| G: -5717.87902 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.92581 HOMO: -6.72393 LUMO: 2.19596 factor:1 | -1 (1.31891) | -1 | -1 |
| G: -5717.87902 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.96781 HOMO: -6.11440 LUMO: 2.10072 factor:1 | -1 (0.27690) | -1 | -1 |
| G: -5717.87902 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.80639 HOMO: -6.34297 LUMO: 1.92657 factor:1 | -1 (0.43832) | -1 | -1 |
| G: -5717.87902 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.00760 HOMO: -6.24773 LUMO: 2.00276 factor:1 | -1 (1.23711) | -1 | -1 |
| G: -5717.87902 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.85057 HOMO: -6.75114 LUMO: 1.98643 factor:1 | -1 (1.39415) | -1 | -1 |
| G: -5717.87902 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.80172 HOMO: -6.69128 LUMO: 2.08711 factor:1 | -1 (1.44299) | -1 | -1 |
| G: -5717.87902 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.54389 HOMO: -6.65318 LUMO: 2.15514 factor:1 | -1 (1.70082) | -1 | -1 |
| G: -5717.87902 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.88797 HOMO: -6.67495 LUMO: 1.72248 factor:1 | -1 (0.35674) | -1 | -1 |
| G: -5717.87902 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.77407 HOMO: -6.58243 LUMO: 1.83405 factor:1 | -1 (0.47065) | -1 | -1 |
| G: -5717.87902 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.38418 HOMO: -6.61237 LUMO: 1.69799 factor:1 | -1 (0.86053) | -1 | -1 |
| G: -5717.87902 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.99304 HOMO: -6.57427 LUMO: 2.29936 factor:1 | -1 (0.25168) | -1 | -1 |
| G: -5717.87902 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.87694 HOMO: -6.40012 LUMO: 2.35378 factor:1 | 1 (-0.63223) | -1 | -1 |
| G: -5717.87902 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11983.42923 HOMO: -6.90081 LUMO: 2.26671 factor:1 | 1 (-1.18451) | -1 | -1 |
| G: -5717.87902 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11983.50983 HOMO: -6.44910 LUMO: 2.25855 factor:1 | 1 (-1.26511) | -1 | -1 |
| G: -5717.87902 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.39972 HOMO: -6.61509 LUMO: 2.26943 factor:1 | -1 (0.84500) | -1 | -1 |
| G: -5717.87902 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11983.51698 HOMO: -6.78924 LUMO: 2.09256 factor:1 | 1 (-1.27227) | -1 | -1 |
| G: -5717.87902 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.12507 HOMO: -6.47087 LUMO: 1.97555 factor:1 | -1 (0.11965) | -1 | -1 |
| G: -5717.87902 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.33674 HOMO: -6.75931 LUMO: 1.98643 factor:1 | 1 (-0.09203) | -1 | -1 |
| G: -5717.87902 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.38238 HOMO: -6.17971 LUMO: 2.09800 factor:1 | 1 (-0.13766) | -1 | -1 |
| G: -5717.87902 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11983.07374 HOMO: -6.83006 LUMO: 1.91840 factor:1 | 1 (-0.82902) | -1 | -1 |
| G: -5717.87902 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.40532 HOMO: -6.72938 LUMO: 2.17419 factor:1 | 1 (-0.16060) | -1 | -1 |
| G: -5717.87902 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11983.09581 HOMO: -6.78924 LUMO: 2.42726 factor:1 | 1 (-0.85109) | -1 | -1 |
| G: -5717.87902 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.56956 HOMO: -6.41372 LUMO: 1.93745 factor:1 | 1 (-0.32485) | -1 | -1 |
| G: -5717.87902 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.56886 HOMO: -6.85455 LUMO: 2.14970 factor:1 | 1 (-0.32414) | -1 | -1 |
| G: -5717.87902 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.71169 HOMO: -6.38651 LUMO: 2.18507 factor:1 | 1 (-0.46697) | -1 | -1 |
| G: -5717.87902 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.61152 HOMO: -6.81373 LUMO: 2.00548 factor:1 | 1 (-0.36681) | -1 | -1 |
| G: -5717.87902 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.47626 HOMO: -6.64774 LUMO: 2.41365 factor:1 | 1 (-0.23154) | -1 | -1 |
| G: -5717.87902 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11983.11948 HOMO: -6.70489 LUMO: 2.31569 factor:1 | 1 (-0.87476) | -1 | -1 |
| G: -5717.87902 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11983.18215 HOMO: -6.49264 LUMO: 1.78779 factor:1 | 1 (-0.93743) | -1 | -1 |
| G: -5717.87902 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.99833 HOMO: -6.81101 LUMO: 1.86670 factor:1 | 1 (-0.75362) | -1 | -1 |
| G: -5717.87902 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.85074 HOMO: -6.72121 LUMO: 1.48846 factor:1 | 1 (-0.60602) | -1 | -1 |
| G: -5717.87902 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11983.23603 HOMO: -6.35930 LUMO: 1.78507 factor:1 | 1 (-0.99131) | -1 | -1 |
| G: -5717.87902 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11983.20392 HOMO: -6.38651 LUMO: 2.04358 factor:1 | 1 (-0.95920) | -1 | -1 |
| G: -5717.87902 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.36703 HOMO: -6.42189 LUMO: 1.99187 factor:1 | 1 (-0.12232) | -1 | -1 |
| G: -5717.87902 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.55713 HOMO: -6.69400 LUMO: 1.61091 factor:1 | 1 (-0.31241) | -1 | -1 |
| G: -5717.87902 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.68538 HOMO: -6.81101 LUMO: 2.17419 factor:1 | 1 (-0.44066) | -1 | -1 |
| G: -5717.87902 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.60954 HOMO: -6.90897 LUMO: 2.28576 factor:1 | 1 (-0.36482) | -1 | -1 |
| G: -5717.87902 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.59367 HOMO: -6.75387 LUMO: 2.31297 factor:1 | 1 (-0.34896) | -1 | -1 |
| G: -5717.87902 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.68843 HOMO: -7.05863 LUMO: 2.18780 factor:1 | -1 (0.55628) | -1 | -1 |
| G: -5717.87902 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.42877 HOMO: -6.56611 LUMO: 1.99187 factor:1 | 1 (-0.18406) | -1 | -1 |
| G: -5717.87902 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.44739 HOMO: -6.59060 LUMO: 1.86398 factor:1 | 1 (-0.20267) | -1 | -1 |
| G: -5717.87902 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.30050 HOMO: -6.59060 LUMO: 1.59459 factor:1 | 1 (-0.05578) | -1 | -1 |
| G: -5717.87902 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.48333 HOMO: -6.57699 LUMO: 1.48030 factor:1 | 1 (-0.23862) | -1 | -1 |
| G: -5717.87902 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.48080 HOMO: -6.99605 LUMO: 2.30208 factor:1 | 1 (-0.23609) | -1 | -1 |
| G: -5717.87902 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.58875 HOMO: -6.42189 LUMO: 2.20412 factor:1 | 1 (-0.34403) | -1 | -1 |
| G: -5717.87902 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.02896 HOMO: -7.15115 LUMO: 1.83405 factor:1 | -1 (0.21576) | 1 | 1 |
| G: -5717.87902 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.67732 HOMO: -7.08040 LUMO: 2.21773 factor:1 | 1 (-0.43261) | 1 | 1 |
| G: -5717.87902 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11983.13322 HOMO: -6.72121 LUMO: 1.89663 factor:1 | 1 (-0.88851) | -1 | -1 |
| G: -5717.87902 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.99284 HOMO: -6.25590 LUMO: 1.85037 factor:1 | 1 (-0.74812) | -1 | -1 |
| G: -5717.87902 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.98938 HOMO: -6.70489 LUMO: 1.98915 factor:1 | 1 (-0.74467) | -1 | -1 |
| G: -5717.87902 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11983.06887 HOMO: -6.53617 LUMO: 2.08439 factor:1 | 1 (-0.82415) | -1 | -1 |
| G: -5717.87902 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.26116 HOMO: -6.69944 LUMO: 1.98915 factor:1 | -1 (0.98356) | -1 | -1 |
| G: -5717.87902 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.00480 HOMO: -6.79468 LUMO: 1.96466 factor:1 | -1 (1.23991) | -1 | -1 |
| G: -5717.87902 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.49729 HOMO: -6.79468 LUMO: 1.99459 factor:1 | 1 (-0.25258) | -1 | -1 |
| G: -5717.87902 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11983.13151 HOMO: -6.58788 LUMO: 1.98371 factor:1 | 1 (-0.88679) | -1 | -1 |
| G: -5717.87902 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11983.29099 HOMO: -6.58788 LUMO: 2.16603 factor:1 | 1 (-1.04628) | -1 | -1 |
| G: -5717.87902 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.52595 HOMO: -6.56883 LUMO: 1.64085 factor:1 | -1 (0.71876) | -1 | -1 |
| G: -5717.87902 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.18629 HOMO: -7.19197 LUMO: 2.66127 factor:1 | -1 (0.05842) | 1 | 1 |
| G: -5717.87902 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.49901 HOMO: -6.48175 LUMO: 2.40004 factor:1 | 1 (-0.25429) | -1 | -1 |
| G: -5717.87902 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.22061 HOMO: -6.18515 LUMO: 2.27759 factor:1 | -1 (0.02411) | -1 | -1 |
| G: -5717.87902 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.42254 HOMO: -6.64774 LUMO: 2.13337 factor:1 | 1 (-0.17783) | -1 | -1 |
| G: -5717.87902 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.89131 HOMO: -6.39740 LUMO: 1.95106 factor:1 | 1 (-0.64660) | -1 | -1 |
| G: -5717.87902 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.93877 HOMO: -6.59332 LUMO: 1.81772 factor:1 | 1 (-0.69405) | -1 | -1 |
| G: -5717.87902 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.52586 HOMO: -6.68312 LUMO: 2.41909 factor:1 | 1 (-0.28115) | -1 | -1 |
| G: -5717.87902 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.52369 HOMO: -5.87494 LUMO: 2.18235 factor:1 | 1 (-0.27897) | -1 | -1 |
| G: -5717.87902 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.57232 HOMO: -6.30488 LUMO: 2.04902 factor:1 | -1 (0.67239) | -1 | -1 |
| G: -5717.87902 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.28806 HOMO: -6.65046 LUMO: 2.05446 factor:1 | 1 (-0.04335) | -1 | -1 |
| G: -5717.87902 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.82794 HOMO: -6.55794 LUMO: 2.06807 factor:1 | 1 (-0.58322) | -1 | -1 |
| G: -5717.87902 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.47803 HOMO: -6.68040 LUMO: 1.99187 factor:1 | 1 (-0.23331) | -1 | -1 |
| G: -5717.87902 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.59743 HOMO: -6.60965 LUMO: 2.18780 factor:1 | 1 (-0.35271) | -1 | -1 |
| G: -5717.87902 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.22959 HOMO: -6.88176 LUMO: 2.10344 factor:1 | -1 (0.01513) | -1 | -1 |
| G: -5717.87902 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.36621 HOMO: -6.63414 LUMO: 1.70615 factor:1 | 1 (-0.12150) | -1 | -1 |
| G: -5717.87902 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.44510 HOMO: -7.15115 LUMO: 2.07351 factor:1 | 1 (-0.20038) | 1 | 1 |
| G: -5717.87902 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.19693 HOMO: -6.85727 LUMO: 2.27759 factor:1 | -1 (0.04778) | -1 | -1 |
| G: -5717.87902 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.88995 HOMO: -6.91713 LUMO: 2.28848 factor:1 | 1 (-0.64524) | -1 | -1 |
| G: -5717.87902 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11983.05395 HOMO: -7.10217 LUMO: 2.14698 factor:1 | 1 (-0.80924) | 1 | 1 |
| G: -5717.87902 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.90628 HOMO: -6.78108 LUMO: 2.45447 factor:1 | 1 (-0.66156) | -1 | -1 |
| G: -5717.87902 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11983.60458 HOMO: -6.78380 LUMO: 2.43542 factor:1 | 1 (-1.35986) | -1 | -1 |
| G: -5717.87902 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11983.01806 HOMO: -6.60965 LUMO: 2.33474 factor:1 | 1 (-0.77335) | -1 | -1 |
| G: -5717.87902 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.91637 HOMO: -6.72665 LUMO: 2.25855 factor:1 | 1 (-0.67166) | -1 | -1 |
| G: -5717.87902 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.73536 HOMO: -6.27495 LUMO: 2.04358 factor:1 | 1 (-0.49065) | -1 | -1 |
| G: -5717.87902 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.60049 HOMO: -6.17426 LUMO: 1.45853 factor:1 | -1 (0.64423) | -1 | -1 |
| G: -5717.87902 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.61357 HOMO: -7.21374 LUMO: 2.33474 factor:1 | -1 (0.63114) | 1 | 1 |
| G: -5717.87902 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.39212 HOMO: -6.94707 LUMO: 1.81772 factor:1 | 1 (-0.14740) | -1 | -1 |
| G: -5717.87902 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.32102 HOMO: -6.80829 LUMO: 0.17960 factor:1 | 1 (-0.07630) | -1 | -1 |
| G: -5717.87902 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.22526 HOMO: -7.19469 LUMO: 1.60819 factor:1 | -1 (0.01946) | 1 | 1 |
| G: -5717.87902 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.21369 HOMO: -6.78652 LUMO: 0.53334 factor:1 | -1 (0.03102) | -1 | -1 |
| G: -5717.87902 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.19810 HOMO: -6.70489 LUMO: 0.74559 factor:1 | -1 (0.04661) | -1 | -1 |
| G: -5717.87902 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.41049 HOMO: -6.72393 LUMO: 0.88981 factor:1 | 1 (-0.16577) | -1 | -1 |
| G: -5717.87902 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.35990 HOMO: -4.54430 LUMO: -0.90614 factor:1 | 1 (-0.11519) | -1 | -1 |
| G: -5717.87902 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.81243 HOMO: -6.83006 LUMO: 0.47348 factor:1 | 1 (-0.56771) | -1 | -1 |
| G: -5717.87902 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.32134 HOMO: -7.07496 LUMO: 0.50613 factor:1 | 1 (-0.07663) | -1 | -1 |
| G: -5717.87902 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.31710 HOMO: -6.62053 LUMO: 0.74559 factor:1 | 1 (-0.07238) | -1 | -1 |
| G: -5717.87902 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.40250 HOMO: -6.79196 LUMO: 1.80139 factor:1 | -1 (0.84222) | -1 | -1 |
| G: -5717.87902 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.39229 HOMO: -6.71033 LUMO: 0.40817 factor:1 | -1 (0.85242) | -1 | -1 |
| G: -5717.87902 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.27441 HOMO: -6.74026 LUMO: 0.95784 factor:1 | -1 (0.97030) | -1 | -1 |
| G: -5717.87902 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.30306 HOMO: -7.34707 LUMO: 0.40001 factor:1 | 1 (-0.05834) | -1 | -1 |
| G: -5717.87902 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.10626 HOMO: -6.19875 LUMO: -0.88709 factor:1 | -1 (0.13845) | -1 | -1 |
| G: -5717.87902 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.34300 HOMO: -6.48719 LUMO: -0.14694 factor:1 | 1 (-0.09829) | -1 | -1 |
| G: -5717.87902 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.16463 HOMO: -6.73482 LUMO: -0.01633 factor:1 | -1 (0.08008) | -1 | -1 |
| G: -5717.87902 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.17075 HOMO: -7.05591 LUMO: -0.20136 factor:1 | -1 (0.07396) | -1 | -1 |
| G: -5717.87902 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.77017 HOMO: -6.38651 LUMO: -2.07895 factor:1 | 1 (-0.52545) | -1 | -1 |
| G: -5717.87902 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.31225 HOMO: -6.85455 LUMO: -1.03403 factor:1 | 1 (-0.06754) | -1 | -1 |
| G: -5717.87902 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.08463 HOMO: -6.72121 LUMO: -0.99322 factor:1 | -1 (0.16008) | -1 | -1 |
| G: -5717.87902 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.20730 HOMO: -6.53890 LUMO: -0.10885 factor:1 | -1 (0.03742) | -1 | -1 |
| G: -5717.87902 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.19767 HOMO: -6.68312 LUMO: 0.21225 factor:1 | -1 (0.04705) | -1 | -1 |
| G: -5717.87902 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.74753 HOMO: -6.68040 LUMO: 0.21225 factor:1 | 1 (-0.50281) | -1 | -1 |
| G: -5717.87902 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11983.54349 HOMO: -6.76475 LUMO: -0.64491 factor:1 | 1 (-1.29877) | -1 | -1 |
| G: -5717.87902 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11983.55219 HOMO: -6.48175 LUMO: 0.41633 factor:1 | 1 (-1.30748) | -1 | -1 |
| G: -5717.87902 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.56058 HOMO: -6.42733 LUMO: 0.16599 factor:1 | 1 (-0.31587) | -1 | -1 |
| G: -5717.87902 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.36391 HOMO: -6.66679 LUMO: 0.77825 factor:1 | -1 (0.88081) | -1 | -1 |
| G: -5717.87902 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.08665 HOMO: -6.75931 LUMO: -0.73471 factor:1 | -1 (1.15806) | -1 | -1 |
| G: -5717.87902 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.18452 HOMO: -6.53617 LUMO: 0.38096 factor:1 | -1 (0.06019) | -1 | -1 |
| G: -5717.87902 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.87728 HOMO: -6.34297 LUMO: 0.35375 factor:1 | -1 (0.36744) | -1 | -1 |
| G: -5717.87902 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.22186 HOMO: -7.11850 LUMO: -0.03265 factor:1 | -1 (0.02286) | -1 | -1 |
| G: -5717.87902 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.06874 HOMO: -5.21914 LUMO: 1.29798 factor:1 | -1 (0.17598) | -1 | -1 |
| G: -5717.87902 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.99755 HOMO: -7.09129 LUMO: -0.66668 factor:1 | -1 (0.24716) | -1 | -1 |
| G: -5717.87902 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.71142 HOMO: -6.96884 LUMO: -0.31021 factor:1 | 1 (-0.46670) | -1 | -1 |
| G: -5717.87902 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.06708 HOMO: -6.51713 LUMO: -0.59865 factor:1 | -1 (0.17764) | -1 | -1 |
| G: -5717.87902 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.15130 HOMO: -6.69400 LUMO: -0.07075 factor:1 | -1 (0.09342) | -1 | -1 |
| G: -5717.87902 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.12278 HOMO: -5.28173 LUMO: 1.17281 factor:1 | -1 (0.12193) | -1 | -1 |
| G: -5717.87902 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.44831 HOMO: -6.54434 LUMO: 0.32109 factor:1 | 1 (-0.20360) | -1 | -1 |
| G: -5717.87902 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11983.26084 HOMO: -6.79740 LUMO: -0.24762 factor:1 | 1 (-1.01613) | -1 | -1 |
| G: -5717.87902 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.40031 HOMO: -6.91986 LUMO: -0.14694 factor:1 | 1 (-0.15559) | -1 | -1 |
| G: -5717.87902 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11983.16827 HOMO: -6.75114 LUMO: 0.18504 factor:1 | 1 (-0.92355) | -1 | -1 |
| G: -5717.87902 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11983.22552 HOMO: -6.74842 LUMO: 0.69389 factor:1 | 1 (-0.98081) | -1 | -1 |
| G: -5717.87902 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.38062 HOMO: -7.01782 LUMO: 0.56600 factor:1 | -1 (0.86410) | -1 | -1 |
| G: -5717.87902 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.34153 HOMO: -6.47359 LUMO: -0.56600 factor:1 | 1 (-0.09682) | -1 | -1 |
| G: -5717.87902 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.32330 HOMO: -6.63686 LUMO: -0.55783 factor:1 | 1 (-0.07859) | -1 | -1 |
| G: -5717.87902 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.35693 HOMO: -4.13885 LUMO: -2.05446 factor:1 | 1 (-0.11222) | -1 | -1 |
| G: -5717.87902 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.39307 HOMO: -6.34570 LUMO: 0.19864 factor:1 | 1 (-0.14836) | -1 | -1 |
| G: -5717.87902 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.35185 HOMO: -6.47903 LUMO: 0.24762 factor:1 | 1 (-0.10713) | -1 | -1 |
| G: -5717.87902 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.45634 HOMO: -6.15249 LUMO: 0.32109 factor:1 | 1 (-0.21162) | -1 | -1 |
| G: -5717.87902 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.61191 HOMO: -6.84366 LUMO: 0.29116 factor:1 | -1 (0.63280) | -1 | -1 |
| G: -5717.87902 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.80185 HOMO: -6.34297 LUMO: 0.19864 factor:1 | -1 (0.44287) | -1 | -1 |
| G: -5717.87902 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11983.40533 HOMO: -6.51168 LUMO: 0.30749 factor:1 | 1 (-1.16062) | -1 | -1 |
| G: -5717.87902 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11983.02438 HOMO: -6.79468 LUMO: -0.16599 factor:1 | 1 (-0.77966) | -1 | -1 |
| G: -5717.87902 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.27571 HOMO: -7.24095 LUMO: 0.15238 factor:1 | 1 (-0.03099) | -1 | -1 |
| G: -5717.87902 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.79009 HOMO: -7.06952 LUMO: -0.34558 factor:1 | 1 (-0.54537) | -1 | -1 |
| G: -5717.87902 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.42658 HOMO: -6.88176 LUMO: 0.02177 factor:1 | -1 (0.81814) | -1 | -1 |
| G: -5717.87902 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.41155 HOMO: -6.37291 LUMO: -0.69117 factor:1 | 1 (-0.16683) | -1 | -1 |
| G: -5717.87902 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.02112 HOMO: -6.83278 LUMO: -0.59049 factor:1 | -1 (0.22360) | -1 | -1 |
| G: -5717.87902 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.58537 HOMO: -6.57155 LUMO: -0.33470 factor:1 | 1 (-0.34066) | -1 | -1 |
| G: -5717.87902 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.63074 HOMO: -6.89537 LUMO: -0.58504 factor:1 | -1 (0.61397) | -1 | -1 |
| G: -5717.87902 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.29485 HOMO: -6.57155 LUMO: -0.34831 factor:1 | -1 (0.94987) | -1 | -1 |
| G: -5717.87902 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.23688 HOMO: -6.64774 LUMO: -0.95784 factor:1 | -1 (0.00784) | -1 | -1 |
| G: -5717.87902 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.54434 HOMO: -6.91713 LUMO: -0.69933 factor:1 | 1 (-0.29962) | -1 | -1 |
| G: -5717.87902 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.89393 HOMO: -6.80557 LUMO: -0.65035 factor:1 | -1 (0.35078) | -1 | -1 |
| G: -5717.87902 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.71417 HOMO: -7.26544 LUMO: -0.79729 factor:1 | -1 (0.53054) | -1 | -1 |
| G: -5717.87902 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.29625 HOMO: -6.69128 LUMO: -0.16871 factor:1 | 1 (-0.05154) | -1 | -1 |
| G: -5717.87902 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.62412 HOMO: -6.88448 LUMO: 0.13061 factor:1 | 1 (-0.37941) | -1 | -1 |
| G: -5717.87902 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11983.12479 HOMO: -6.50352 LUMO: 0.12245 factor:1 | 1 (-0.88007) | -1 | -1 |
| G: -5717.87902 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.41756 HOMO: -6.56067 LUMO: 0.17687 factor:1 | 1 (-0.17285) | -1 | -1 |
| G: -5717.87902 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.85747 HOMO: -6.70216 LUMO: 0.25034 factor:1 | -1 (0.38725) | -1 | -1 |
| G: -5717.87902 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.29012 HOMO: -6.51713 LUMO: -0.78369 factor:1 | -1 (1.95459) | -1 | -1 |
| G: -5717.87902 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.22704 HOMO: -6.50352 LUMO: 0.12245 factor:1 | -1 (1.01768) | -1 | -1 |
| G: -5717.87902 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.16821 HOMO: -6.22052 LUMO: -0.83811 factor:1 | -1 (1.07651) | -1 | -1 |
| G: -5717.87902 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.04145 HOMO: -6.51168 LUMO: -0.76464 factor:1 | -1 (1.20326) | -1 | -1 |
| G: -5717.87902 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.92634 HOMO: -7.14571 LUMO: -0.80274 factor:1 | -1 (0.31837) | -1 | -1 |
| G: -5717.87902 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.04137 HOMO: -6.66679 LUMO: -0.88709 factor:1 | -1 (1.20334) | -1 | -1 |
| G: -5717.87902 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.67475 HOMO: -6.76203 LUMO: -1.43948 factor:1 | -1 (0.56997) | -1 | -1 |
| G: -5717.87902 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.10121 HOMO: -6.57427 LUMO: -1.62996 factor:1 | -1 (1.14350) | -1 | -1 |
| G: -5717.87902 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.79302 HOMO: -5.05043 LUMO: 1.24900 factor:1 | 1 (-0.54831) | -1 | -1 |
| G: -5717.87902 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.07440 HOMO: -6.53345 LUMO: 0.23130 factor:1 | -1 (0.17032) | -1 | -1 |
| G: -5717.87902 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.89482 HOMO: -7.18381 LUMO: -0.22585 factor:1 | 1 (-0.65011) | -1 | -1 |
| G: -5717.87902 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.09742 HOMO: -7.00965 LUMO: -1.79595 factor:1 | -1 (0.14730) | -1 | -1 |
| G: -5717.87902 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.89589 HOMO: -6.08174 LUMO: -0.82995 factor:1 | -1 (0.34882) | -1 | -1 |
| G: -5717.87902 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11983.48033 HOMO: -6.42189 LUMO: -0.84355 factor:1 | 1 (-1.23561) | -1 | -1 |
| G: -5717.87902 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.83365 HOMO: -6.53890 LUMO: 0.60409 factor:1 | 1 (-0.58894) | -1 | -1 |
| G: -5717.87902 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.63613 HOMO: -6.62869 LUMO: 0.43810 factor:1 | -1 (0.60858) | -1 | -1 |
| G: -5717.87902 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.91453 HOMO: -6.68312 LUMO: 0.64491 factor:1 | -1 (0.33018) | -1 | -1 |
| G: -5717.87902 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.92672 HOMO: -6.42189 LUMO: 1.51295 factor:1 | -1 (0.31799) | -1 | -1 |
| G: -5717.87902 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.32521 HOMO: -6.17971 LUMO: 1.67622 factor:1 | -1 (0.91950) | -1 | -1 |
| G: -5717.87902 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.56914 HOMO: -6.79196 LUMO: 1.36873 factor:1 | -1 (0.67558) | -1 | -1 |
| G: -5717.87902 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.91902 HOMO: -7.38517 LUMO: 0.56328 factor:1 | -1 (0.32569) | 1 | 1 |
| G: -5717.87902 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.87875 HOMO: -7.56204 LUMO: 0.71566 factor:1 | -1 (0.36597) | 1 | 1 |
| G: -5717.87902 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.09268 HOMO: -6.45726 LUMO: -1.91840 factor:1 | -1 (0.15203) | -1 | -1 |
| G: -5717.87902 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.23032 HOMO: -6.13073 LUMO: -0.97417 factor:1 | -1 (0.01439) | -1 | -1 |
| G: -5717.87902 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.71635 HOMO: -6.50352 LUMO: -0.69661 factor:1 | -1 (0.52836) | -1 | -1 |
| G: -5717.87902 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.72909 HOMO: -6.76747 LUMO: -1.71976 factor:1 | -1 (0.51563) | -1 | -1 |
| G: -5717.87902 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11983.29309 HOMO: -6.48447 LUMO: -0.89525 factor:1 | 1 (-1.04837) | -1 | -1 |
| G: -5717.87902 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11983.60343 HOMO: -7.11850 LUMO: -0.71566 factor:1 | 1 (-1.35872) | -1 | -1 |
| G: -5717.87902 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11983.73846 HOMO: -6.80285 LUMO: -0.49253 factor:1 | 1 (-1.49374) | -1 | -1 |
| G: -5717.87902 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11983.19502 HOMO: -6.80557 LUMO: -0.88165 factor:1 | 1 (-0.95030) | -1 | -1 |
| G: -5717.87902 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11983.17611 HOMO: -6.94162 LUMO: -0.08980 factor:1 | 1 (-0.93139) | -1 | -1 |
| G: -5717.87902 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.08515 HOMO: -6.97972 LUMO: -0.29388 factor:1 | -1 (0.15957) | -1 | -1 |
| G: -5717.87902 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.48301 HOMO: -6.75114 LUMO: 0.04626 factor:1 | -1 (0.76170) | -1 | -1 |
| G: -5717.87902 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.40886 HOMO: -7.15932 LUMO: 0.68845 factor:1 | -1 (0.83585) | 1 | 1 |
| G: -5717.87902 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.23591 HOMO: -7.36612 LUMO: 0.63675 factor:1 | -1 (1.00881) | 1 | 1 |
| G: -5717.87902 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.26175 HOMO: -7.02598 LUMO: -0.66124 factor:1 | 1 (-0.01703) | -1 | -1 |
| G: -5717.87902 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.80111 HOMO: -6.89264 LUMO: -0.54967 factor:1 | -1 (0.44360) | -1 | -1 |
| G: -5717.87902 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.34771 HOMO: -6.97700 LUMO: 0.27756 factor:1 | 1 (-0.10300) | -1 | -1 |
| G: -5717.87902 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.25062 HOMO: -6.60965 LUMO: 0.08163 factor:1 | 1 (-0.00590) | -1 | -1 |
| G: -5717.87902 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11983.29404 HOMO: -6.70761 LUMO: 0.40001 factor:1 | 1 (-1.04933) | -1 | -1 |
| G: -5717.87902 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.20131 HOMO: -6.69128 LUMO: 0.23674 factor:1 | -1 (0.04340) | -1 | -1 |
| G: -5717.87902 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11983.13143 HOMO: -6.69128 LUMO: -0.69933 factor:1 | 1 (-0.88671) | -1 | -1 |
| G: -5717.87902 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.85327 HOMO: -6.18515 LUMO: -0.85988 factor:1 | 1 (-0.60856) | -1 | -1 |
| G: -5717.87902 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.26847 HOMO: -6.86815 LUMO: -1.90208 factor:1 | 1 (-0.02376) | -1 | -1 |
| G: -5717.87902 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.24063 HOMO: -6.37563 LUMO: -1.74697 factor:1 | -1 (0.00408) | -1 | -1 |
| G: -5717.87902 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.58242 HOMO: -6.75659 LUMO: 0.36463 factor:1 | -1 (0.66230) | -1 | -1 |
| G: -5717.87902 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.69906 HOMO: -6.91441 LUMO: -0.88981 factor:1 | 1 (-0.45435) | -1 | -1 |
| G: -5717.87902 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.65072 HOMO: -6.71305 LUMO: -0.29933 factor:1 | -1 (0.59400) | -1 | -1 |
| G: -5717.87902 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.96166 HOMO: -6.91441 LUMO: -1.04492 factor:1 | -1 (0.28305) | -1 | -1 |
| G: -5717.87902 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.07312 HOMO: -6.05453 LUMO: -0.83539 factor:1 | -1 (0.17160) | -1 | -1 |
| G: -5717.87902 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.25854 HOMO: -7.35252 LUMO: -0.45715 factor:1 | 1 (-0.01382) | -1 | -1 |
| G: -5717.87902 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.90917 HOMO: -6.41644 LUMO: -0.97417 factor:1 | -1 (0.33554) | -1 | -1 |
| G: -5717.87902 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.21843 HOMO: -6.78924 LUMO: 0.36735 factor:1 | -1 (0.02629) | -1 | -1 |
| G: -5717.87902 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11983.17673 HOMO: -6.74298 LUMO: 0.51974 factor:1 | 1 (-0.93202) | -1 | -1 |
| G: -5717.87902 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11983.11730 HOMO: -6.48992 LUMO: 1.44765 factor:1 | 1 (-0.87259) | -1 | -1 |
| G: -5717.87902 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.95919 HOMO: -6.12528 LUMO: 1.57826 factor:1 | -1 (0.28553) | -1 | -1 |
| G: -5717.87902 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.03582 HOMO: -6.62325 LUMO: 1.57826 factor:1 | -1 (1.20889) | -1 | -1 |
| G: -5717.87902 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.93909 HOMO: -6.19875 LUMO: 1.29798 factor:1 | -1 (1.30563) | -1 | -1 |
| G: -5717.87902 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.57990 HOMO: -6.74570 LUMO: 1.52112 factor:1 | -1 (1.66482) | -1 | -1 |
| G: -5717.87902 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.88252 HOMO: -6.84094 LUMO: 1.48574 factor:1 | 1 (-0.63781) | -1 | -1 |
| G: -5717.87902 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.02433 HOMO: -6.85183 LUMO: 0.33470 factor:1 | -1 (0.22039) | -1 | -1 |
| G: -5717.87902 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.68546 HOMO: -6.51168 LUMO: 0.48164 factor:1 | 1 (-0.44074) | -1 | -1 |
| G: -5717.87902 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.61610 HOMO: -6.25046 LUMO: 0.75648 factor:1 | -1 (0.62861) | -1 | -1 |
| G: -5717.87902 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11979.46687 HOMO: -6.65591 LUMO: 0.32109 factor:1 | -1 (2.77785) | -1 | -1 |
| G: -5717.87902 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.04079 HOMO: -6.71033 LUMO: 0.40817 factor:1 | -1 (0.20392) | -1 | -1 |
| G: -5717.87902 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.54377 HOMO: -6.75114 LUMO: 0.73471 factor:1 | 1 (-0.29905) | -1 | -1 |
| G: -5717.87902 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.65172 HOMO: -6.50624 LUMO: 0.59321 factor:1 | -1 (0.59299) | -1 | -1 |
| G: -5717.87902 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.30423 HOMO: -6.39740 LUMO: 0.83267 factor:1 | -1 (0.94048) | -1 | -1 |
| G: -5717.87902 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.32588 HOMO: -6.44094 LUMO: 0.65579 factor:1 | -1 (1.91884) | -1 | -1 |
| G: -5717.87902 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.16639 HOMO: -6.52257 LUMO: 0.05714 factor:1 | -1 (2.07832) | -1 | -1 |
| G: -5717.87902 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.31247 HOMO: -7.10217 LUMO: 0.49797 factor:1 | 1 (-0.06776) | -1 | -1 |
| G: -5717.87902 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.33857 HOMO: -6.83006 LUMO: 0.55783 factor:1 | 1 (-0.09385) | -1 | -1 |
| G: -5717.87902 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.35000 HOMO: -6.99333 LUMO: -0.79457 factor:1 | 1 (-0.10528) | -1 | -1 |
| G: -5717.87902 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.72596 HOMO: -6.64230 LUMO: 0.32382 factor:1 | -1 (0.51876) | -1 | -1 |
| G: -5717.87902 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.46309 HOMO: -6.90897 LUMO: 0.30749 factor:1 | 1 (-0.21837) | -1 | -1 |
| G: -5717.87902 HOMO: -7.26544 LUMO: -1.10478 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.82185 HOMO: -7.09129 LUMO: 1.33336 factor:1 | -1 (0.42286) | 1 | 1 |
| G: -5717.87902 HOMO: -7.26544 LUMO: -1.10478 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.52184 HOMO: -6.66951 LUMO: 1.34424 factor:1 | -1 (0.72287) | -1 | -1 |
| G: -5717.87902 HOMO: -7.26544 LUMO: -1.10478 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.86566 HOMO: -7.02870 LUMO: 1.48574 factor:1 | -1 (0.37905) | -1 | -1 |
| G: -5717.87902 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.25797 HOMO: -7.26544 LUMO: 0.32926 factor:1 | 1 (-0.01325) | -1 | -1 |
| G: -5717.87902 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.37938 HOMO: -6.56067 LUMO: -0.45987 factor:1 | 1 (-0.13467) | -1 | -1 |
| G: -5717.87902 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.56861 HOMO: -6.54434 LUMO: -0.28300 factor:1 | 1 (-0.32390) | -1 | -1 |
| G: -5717.87902 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.32651 HOMO: -7.19469 LUMO: 0.54695 factor:1 | 1 (-0.08180) | -1 | -1 |
| G: -5717.87902 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.61240 HOMO: -6.47359 LUMO: -0.22041 factor:1 | -1 (0.63231) | -1 | -1 |
| G: -5717.87902 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.06463 HOMO: -6.80013 LUMO: 2.08167 factor:1 | -1 (0.18008) | -1 | -1 |
| G: -5717.87902 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.16136 HOMO: -6.23957 LUMO: 1.67894 factor:1 | -1 (2.08336) | -1 | -1 |
| G: -5717.87902 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.28985 HOMO: -6.75114 LUMO: -0.62858 factor:1 | -1 (1.95487) | -1 | -1 |
| G: -5717.87902 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.12265 HOMO: -6.79468 LUMO: -0.64491 factor:1 | -1 (1.12206) | -1 | -1 |
| G: -5717.87902 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.48944 HOMO: -6.84911 LUMO: -0.69661 factor:1 | -1 (0.75528) | -1 | -1 |
| G: -5717.87902 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.03911 HOMO: -7.54028 LUMO: 0.25851 factor:1 | -1 (1.20560) | -1 | -1 |
| G: -5717.87902 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.98430 HOMO: -6.92802 LUMO: -0.71022 factor:1 | -1 (0.26041) | -1 | -1 |
| G: -5717.87902 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.18170 HOMO: -6.72665 LUMO: -0.46804 factor:1 | -1 (1.06301) | -1 | -1 |
| G: -5717.87902 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.11811 HOMO: -6.63686 LUMO: -0.23674 factor:1 | -1 (1.12661) | -1 | -1 |
| G: -5717.87902 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.63078 HOMO: -7.21102 LUMO: 0.54423 factor:1 | -1 (1.61393) | -1 | -1 |
| G: -5717.87902 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.43010 HOMO: -6.63414 LUMO: -0.25034 factor:1 | -1 (1.81462) | -1 | -1 |
| G: -5717.87902 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.26617 HOMO: -6.70761 LUMO: -0.31837 factor:1 | -1 (1.97854) | -1 | -1 |
| G: -5717.87902 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.46623 HOMO: -6.57155 LUMO: 1.76874 factor:1 | -1 (1.77848) | -1 | -1 |
| G: -5717.87902 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.05082 HOMO: -6.84366 LUMO: 2.04358 factor:1 | -1 (1.19390) | -1 | -1 |
| G: -5717.87902 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11979.69694 HOMO: -6.60420 LUMO: 1.80139 factor:1 | -1 (2.54777) | -1 | -1 |
| G: -5717.87902 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.25292 HOMO: -7.03686 LUMO: 2.21229 factor:1 | -1 (1.99179) | -1 | -1 |
| G: -5717.87902 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.23480 HOMO: -6.77564 LUMO: 1.97555 factor:1 | -1 (2.00991) | -1 | -1 |
| G: -5717.87902 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.40894 HOMO: -6.40012 LUMO: 2.17691 factor:1 | 1 (-0.16422) | -1 | -1 |
| G: -5717.87902 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.56687 HOMO: -6.80013 LUMO: 2.25582 factor:1 | 1 (-0.32216) | -1 | -1 |
| G: -5717.87902 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.39408 HOMO: -6.74298 LUMO: 2.31569 factor:1 | 1 (-0.14936) | -1 | -1 |
| G: -5717.87902 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.55755 HOMO: -6.68856 LUMO: 1.85854 factor:1 | -1 (0.68717) | -1 | -1 |
| G: -5717.87902 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.93147 HOMO: -6.17971 LUMO: 1.52928 factor:1 | -1 (1.31325) | -1 | -1 |
| G: -5717.87902 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.52809 HOMO: -6.54162 LUMO: 1.91840 factor:1 | 1 (-0.28338) | -1 | -1 |
| G: -5717.87902 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.95723 HOMO: -6.80013 LUMO: -0.55511 factor:1 | -1 (0.28749) | -1 | -1 |
| G: -5717.87902 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.41474 HOMO: -7.46953 LUMO: 0.28572 factor:1 | -1 (0.82997) | -1 | -1 |
| G: -5717.87902 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.07043 HOMO: -6.61781 LUMO: -0.54967 factor:1 | -1 (0.17429) | -1 | -1 |
| G: -5717.87902 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.31969 HOMO: -6.56339 LUMO: -0.47892 factor:1 | -1 (0.92502) | -1 | -1 |
| G: -5717.87902 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.07575 HOMO: -6.65591 LUMO: -0.25307 factor:1 | -1 (2.16897) | -1 | -1 |
| G: -5717.87902 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11979.40126 HOMO: -6.62869 LUMO: -0.23402 factor:1 | -1 (2.84345) | -1 | -1 |
| G: -5717.87902 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11979.46828 HOMO: -6.58243 LUMO: -0.19048 factor:1 | -1 (2.77643) | -1 | -1 |
| G: -5717.87902 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11978.90525 HOMO: -7.27632 LUMO: 0.52790 factor:1 | -1 (3.33946) | -1 | -1 |
| G: -5717.87902 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.16764 HOMO: -7.21102 LUMO: 0.57688 factor:1 | -1 (2.07707) | -1 | -1 |
| G: -5717.87902 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.43834 HOMO: -6.72393 LUMO: -0.53879 factor:1 | -1 (1.80637) | -1 | -1 |
| G: -5717.87902 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.33148 HOMO: -7.42054 LUMO: -0.99322 factor:1 | -1 (1.91323) | -1 | -1 |
| G: -5717.87902 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.22763 HOMO: -6.88992 LUMO: -0.71838 factor:1 | -1 (0.01709) | -1 | -1 |
| G: -5717.87902 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.38874 HOMO: -6.88176 LUMO: -0.61226 factor:1 | 1 (-0.14403) | -1 | -1 |
| G: -5717.87902 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.83437 HOMO: -7.36340 LUMO: -1.04492 factor:1 | -1 (0.41035) | -1 | -1 |
| G: -5717.87902 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.50143 HOMO: -6.65863 LUMO: -0.41906 factor:1 | 1 (-0.25671) | -1 | -1 |
| G: -5717.87902 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.39367 HOMO: -7.15115 LUMO: -0.66396 factor:1 | 1 (-0.14896) | -1 | -1 |
| G: -5717.87902 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.45141 HOMO: -7.10489 LUMO: -0.64491 factor:1 | 1 (-0.20670) | -1 | -1 |
| G: -5717.87902 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.87135 HOMO: -7.20285 LUMO: 0.47892 factor:1 | -1 (0.37337) | -1 | -1 |
| G: -5717.87902 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.34711 HOMO: -6.55794 LUMO: -0.28844 factor:1 | 1 (-0.10240) | -1 | -1 |
| G: -5717.87902 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.46766 HOMO: -7.19197 LUMO: -0.69661 factor:1 | 1 (-0.22294) | -1 | -1 |
| G: -5717.87902 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.65635 HOMO: -6.56883 LUMO: -0.32926 factor:1 | -1 (0.58836) | -1 | -1 |
| G: -5717.87902 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.18606 HOMO: -6.70761 LUMO: 1.95650 factor:1 | -1 (1.05866) | -1 | -1 |
| G: -5717.87902 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.98808 HOMO: -6.60420 LUMO: 1.80684 factor:1 | -1 (0.25663) | -1 | -1 |
| G: -5717.87902 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.48935 HOMO: -6.84094 LUMO: 1.64085 factor:1 | -1 (0.75536) | -1 | -1 |
| G: -5717.87902 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.18100 HOMO: -6.69128 LUMO: 1.90208 factor:1 | -1 (2.06371) | -1 | -1 |
| G: -5717.87902 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.29048 HOMO: -6.75387 LUMO: 1.70343 factor:1 | 1 (-0.04577) | -1 | -1 |
| G: -5717.87902 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.40453 HOMO: -7.07496 LUMO: 2.10072 factor:1 | 1 (-0.15981) | -1 | -1 |
| G: -5717.87902 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.37176 HOMO: -6.99877 LUMO: 2.24494 factor:1 | 1 (-0.12705) | -1 | -1 |
| G: -5717.87902 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.99140 HOMO: -6.63414 LUMO: 2.17691 factor:1 | -1 (0.25331) | -1 | -1 |
| G: -5717.87902 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.49480 HOMO: -6.44638 LUMO: 1.78235 factor:1 | -1 (0.74992) | -1 | -1 |
| G: -5717.87902 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.11889 HOMO: -6.87632 LUMO: 1.84221 factor:1 | -1 (0.12583) | -1 | -1 |
| G: -5717.87902 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.13423 HOMO: -6.85183 LUMO: 1.68711 factor:1 | -1 (2.11049) | -1 | -1 |
| G: -5717.87902 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.22533 HOMO: -6.96339 LUMO: 2.26671 factor:1 | -1 (2.01938) | -1 | -1 |
| G: -5717.87902 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.04311 HOMO: -6.63141 LUMO: 1.96738 factor:1 | -1 (0.20161) | -1 | -1 |
| G: -5717.87902 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.12418 HOMO: -6.37019 LUMO: 2.23133 factor:1 | -1 (1.12054) | -1 | -1 |
| G: -5717.87902 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.91500 HOMO: -7.11034 LUMO: 2.32385 factor:1 | -1 (1.32971) | 1 | 1 |
| G: -5717.87902 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.18627 HOMO: -6.91986 LUMO: 1.65445 factor:1 | -1 (1.05844) | -1 | -1 |
| G: -5717.87902 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.15142 HOMO: -7.12938 LUMO: 2.28304 factor:1 | -1 (2.09329) | 1 | 1 |
| G: -5717.87902 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.19662 HOMO: -6.54978 LUMO: 1.92112 factor:1 | -1 (2.04809) | -1 | -1 |
| G: -5717.87902 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.57109 HOMO: -6.83006 LUMO: 2.48712 factor:1 | 1 (-0.32637) | -1 | -1 |
| G: -5717.87902 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.18259 HOMO: -6.97972 LUMO: 1.96738 factor:1 | -1 (0.06212) | -1 | -1 |
| G: -5717.87902 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11983.45802 HOMO: -6.69944 LUMO: 2.06262 factor:1 | 1 (-1.21330) | -1 | -1 |
| G: -5717.87902 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.61691 HOMO: -6.76747 LUMO: 2.10888 factor:1 | 1 (-0.37220) | -1 | -1 |
| G: -5717.87902 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11983.37848 HOMO: -6.91169 LUMO: 2.06534 factor:1 | 1 (-1.13376) | -1 | -1 |
| G: -5717.87902 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.46173 HOMO: -7.03414 LUMO: 1.93473 factor:1 | 1 (-0.21701) | -1 | -1 |
| G: -5717.87902 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.56475 HOMO: -7.03142 LUMO: 2.52250 factor:1 | 1 (-0.32003) | -1 | -1 |
| G: -5717.87902 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11983.19192 HOMO: -6.34025 LUMO: 2.61229 factor:1 | 1 (-0.94720) | -1 | -1 |
| G: -5717.87902 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11983.08122 HOMO: -6.98788 LUMO: 2.28304 factor:1 | 1 (-0.83651) | -1 | -1 |
| G: -5717.87902 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.33459 HOMO: -6.97700 LUMO: 2.53882 factor:1 | 1 (-0.08988) | -1 | -1 |
| G: -5717.87902 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.58167 HOMO: -6.58788 LUMO: 1.94289 factor:1 | 1 (-0.33696) | -1 | -1 |
| G: -5717.87902 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.28174 HOMO: -6.78652 LUMO: 2.13609 factor:1 | -1 (1.96297) | -1 | -1 |
| G: -5717.87902 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.05935 HOMO: -6.55250 LUMO: 1.82861 factor:1 | -1 (0.18536) | -1 | -1 |
| G: -5717.87902 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.72681 HOMO: -6.45998 LUMO: 1.75786 factor:1 | -1 (1.51791) | -1 | -1 |
| G: -5717.87902 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.99193 HOMO: -6.78924 LUMO: 2.33746 factor:1 | -1 (1.25279) | -1 | -1 |
| G: -5717.87902 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.20847 HOMO: -6.85727 LUMO: 1.76058 factor:1 | -1 (0.03625) | -1 | -1 |
| G: -5717.87902 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.99826 HOMO: -6.70489 LUMO: 1.84493 factor:1 | -1 (0.24645) | -1 | -1 |
| G: -5717.87902 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.29489 HOMO: -6.71305 LUMO: 1.53472 factor:1 | 1 (-0.05018) | -1 | -1 |
| G: -5717.87902 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11983.30073 HOMO: -6.76747 LUMO: 1.48846 factor:1 | 1 (-1.05602) | -1 | -1 |
| G: -5717.87902 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11983.18530 HOMO: -6.69128 LUMO: 1.95922 factor:1 | 1 (-0.94059) | -1 | -1 |
| G: -5717.87902 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.47351 HOMO: -6.67495 LUMO: 2.05446 factor:1 | 1 (-0.22879) | -1 | -1 |
| G: -5717.87902 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.40455 HOMO: -6.63686 LUMO: 2.25310 factor:1 | 1 (-0.15984) | -1 | -1 |
| G: -5717.87902 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.56405 HOMO: -6.63958 LUMO: 2.14154 factor:1 | -1 (0.68067) | -1 | -1 |
| G: -5717.87902 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.20833 HOMO: -6.62597 LUMO: 2.01908 factor:1 | -1 (0.03638) | -1 | -1 |
| G: -5717.87902 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.89188 HOMO: -7.07768 LUMO: 2.14154 factor:1 | 1 (-0.64717) | -1 | -1 |
| G: -5717.87902 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.49752 HOMO: -6.19603 LUMO: 2.01092 factor:1 | -1 (0.74720) | -1 | -1 |
| G: -5717.87902 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.15065 HOMO: -6.65046 LUMO: 2.15786 factor:1 | -1 (0.09407) | -1 | -1 |
| G: -5717.87902 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11983.10680 HOMO: -6.92258 LUMO: 2.31841 factor:1 | 1 (-0.86208) | -1 | -1 |
| G: -5717.87902 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.95298 HOMO: -6.90081 LUMO: 2.19324 factor:1 | -1 (0.29173) | -1 | -1 |
| G: -5717.87902 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11983.51521 HOMO: -6.85455 LUMO: 1.95650 factor:1 | 1 (-1.27050) | -1 | -1 |
| G: -5717.87902 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11983.59181 HOMO: -6.57699 LUMO: 1.76058 factor:1 | 1 (-1.34710) | -1 | -1 |
| G: -5717.87902 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.14311 HOMO: -6.90625 LUMO: 1.97555 factor:1 | -1 (0.10161) | -1 | -1 |
| G: -5717.87902 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.25244 HOMO: -6.97428 LUMO: 1.92929 factor:1 | 1 (-0.00773) | -1 | -1 |
| G: -5717.87902 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.28594 HOMO: -6.61781 LUMO: -0.41906 factor:1 | 1 (-0.04123) | -1 | -1 |
| G: -5717.87902 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.28948 HOMO: -6.62869 LUMO: -0.81906 factor:1 | 1 (-0.04476) | -1 | -1 |
| G: -5717.87902 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.67189 HOMO: -7.01237 LUMO: 2.00548 factor:1 | -1 (0.57283) | -1 | -1 |
| G: -5717.87902 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.77379 HOMO: -6.85727 LUMO: 2.17691 factor:1 | -1 (0.47092) | -1 | -1 |
| G: -5717.87902 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.88240 HOMO: -6.71849 LUMO: 1.58914 factor:1 | -1 (1.36231) | -1 | -1 |
| G: -5717.87902 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11983.45706 HOMO: -7.52395 LUMO: 0.27211 factor:1 | 1 (-1.21235) | -1 | -1 |
| G: -5717.87902 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11983.04201 HOMO: -6.96611 LUMO: -0.72654 factor:1 | 1 (-0.79729) | -1 | -1 |
| G: -5717.87902 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11983.24778 HOMO: -6.89537 LUMO: -0.68028 factor:1 | 1 (-1.00307) | -1 | -1 |
| G: -5717.87902 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.95459 HOMO: -6.84911 LUMO: -0.58504 factor:1 | -1 (0.29013) | -1 | -1 |
| G: -5717.87902 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.20665 HOMO: -6.79196 LUMO: -0.55783 factor:1 | -1 (0.03807) | -1 | -1 |
| G: -5717.87902 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.34959 HOMO: -6.67767 LUMO: 1.79323 factor:1 | 1 (-0.10487) | -1 | -1 |
| G: -5717.87902 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11983.02487 HOMO: -6.54434 LUMO: 1.91024 factor:1 | 1 (-0.78015) | -1 | -1 |
| G: -5717.87902 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.05598 HOMO: -6.62869 LUMO: 1.69799 factor:1 | -1 (0.18874) | -1 | -1 |
| G: -5717.87902 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.32481 HOMO: -6.72393 LUMO: 2.12249 factor:1 | -1 (0.91991) | -1 | -1 |
| G: -5717.87902 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.42785 HOMO: -6.66407 LUMO: 2.05990 factor:1 | 1 (-0.18313) | -1 | -1 |
| G: -5717.87902 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.87505 HOMO: -7.00149 LUMO: 1.82044 factor:1 | -1 (0.36967) | -1 | -1 |
| G: -5717.87902 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.46273 HOMO: -7.12122 LUMO: 2.16058 factor:1 | 1 (-0.21802) | 1 | 1 |
| G: -5717.87902 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.42797 HOMO: -6.63141 LUMO: 2.21229 factor:1 | -1 (0.81675) | -1 | -1 |
| G: -5717.87902 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.55482 HOMO: -6.37835 LUMO: 2.32113 factor:1 | -1 (0.68989) | -1 | -1 |
| G: -5717.87902 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.29520 HOMO: -6.99605 LUMO: 2.00548 factor:1 | -1 (0.94951) | -1 | -1 |
| G: -5717.87902 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.83974 HOMO: -6.85999 LUMO: 2.39460 factor:1 | -1 (1.40498) | -1 | -1 |
| G: -5717.87902 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.32447 HOMO: -6.85727 LUMO: 2.48712 factor:1 | 1 (-0.07976) | -1 | -1 |
| G: -5717.87902 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.20213 HOMO: -7.04231 LUMO: 2.40277 factor:1 | -1 (0.04259) | -1 | -1 |
| G: -5717.87902 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.17290 HOMO: -6.60692 LUMO: 2.26671 factor:1 | -1 (0.07181) | -1 | -1 |
| G: -5717.87902 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.21734 HOMO: -6.67495 LUMO: 2.14698 factor:1 | -1 (0.02737) | -1 | -1 |
| G: -5717.87902 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.54250 HOMO: -6.73210 LUMO: 2.06807 factor:1 | -1 (0.70222) | -1 | -1 |
| G: -5717.87902 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.42268 HOMO: -7.20013 LUMO: 2.02181 factor:1 | 1 (-0.17796) | 1 | 1 |
| G: -5717.87902 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.76345 HOMO: -7.18653 LUMO: 2.29936 factor:1 | -1 (0.48126) | 1 | 1 |
| G: -5717.87902 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.59553 HOMO: -6.92802 LUMO: 2.36195 factor:1 | -1 (0.64918) | -1 | -1 |
| G: -5717.87902 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.53087 HOMO: -6.89537 LUMO: 1.78779 factor:1 | 1 (-0.28615) | -1 | -1 |
| G: -5717.87902 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.13609 HOMO: -6.96067 LUMO: 2.31297 factor:1 | -1 (0.10863) | -1 | -1 |
| G: -5717.87902 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.58280 HOMO: -6.91441 LUMO: 2.50345 factor:1 | -1 (0.66192) | -1 | -1 |
| G: -5717.87902 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.60453 HOMO: -7.17292 LUMO: 2.12521 factor:1 | 1 (-0.35982) | 1 | 1 |
| G: -5717.87902 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.10425 HOMO: -6.93618 LUMO: 2.35106 factor:1 | -1 (0.14047) | -1 | -1 |
| G: -5717.87902 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11983.08106 HOMO: -6.75931 LUMO: 1.61908 factor:1 | 1 (-0.83634) | -1 | -1 |
| G: -5717.87902 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.35370 HOMO: -6.35930 LUMO: 1.23540 factor:1 | 1 (-0.10898) | -1 | -1 |
| G: -5717.87902 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.88289 HOMO: -6.17971 LUMO: 1.84493 factor:1 | -1 (0.36183) | -1 | -1 |
| G: -5717.87902 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.07453 HOMO: -6.72665 LUMO: 2.61229 factor:1 | -1 (0.17018) | -1 | -1 |
| G: -5717.87902 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.91799 HOMO: -6.62869 LUMO: 2.28304 factor:1 | -1 (0.32673) | -1 | -1 |
| G: -5717.87902 HOMO: -8.88180 LUMO: 1.02315 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.76337 HOMO: -6.58243 LUMO: 0.28028 factor:1 | -1 (0.48134) | -1 | -1 |
| G: -5717.87902 HOMO: -8.88180 LUMO: 1.02315 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.91233 HOMO: -6.79468 LUMO: 0.14966 factor:1 | -1 (0.33239) | -1 | -1 |
| G: -5717.87902 HOMO: -8.88180 LUMO: 1.02315 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.27894 HOMO: -6.63141 LUMO: 0.31021 factor:1 | -1 (1.96578) | -1 | -1 |
| G: -5717.87902 HOMO: -8.88180 LUMO: 1.02315 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.28977 HOMO: -6.81101 LUMO: 0.13878 factor:1 | -1 (1.95495) | -1 | -1 |
| G: -5717.87902 HOMO: -8.88180 LUMO: 1.02315 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.18808 HOMO: -6.72665 LUMO: 0.65579 factor:1 | -1 (2.05664) | -1 | -1 |
| G: -5717.87902 HOMO: -8.88180 LUMO: 1.02315 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.26555 HOMO: -6.53073 LUMO: 0.91430 factor:1 | -1 (1.97917) | -1 | -1 |
| G: -5717.87902 HOMO: -8.88180 LUMO: 1.02315 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.22517 HOMO: -7.19197 LUMO: 1.62996 factor:1 | -1 (2.01955) | 1 | 1 |
| G: -5717.87902 HOMO: -8.88180 LUMO: 1.02315 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11979.90290 HOMO: -6.69400 LUMO: 0.84627 factor:1 | -1 (2.34181) | -1 | -1 |
| G: -5717.87902 HOMO: -8.88180 LUMO: 1.02315 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.13507 HOMO: -6.76475 LUMO: 0.51974 factor:1 | -1 (2.10964) | -1 | -1 |
| G: -5717.87902 HOMO: -8.88180 LUMO: 1.02315 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.10936 HOMO: -6.67767 LUMO: 0.52246 factor:1 | -1 (2.13536) | -1 | -1 |
| G: -5717.87902 HOMO: -8.88180 LUMO: 1.02315 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11979.99776 HOMO: -6.73210 LUMO: 0.94424 factor:1 | -1 (2.24695) | -1 | -1 |
| G: -5717.87902 HOMO: -8.88180 LUMO: 1.02315 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.34077 HOMO: -6.97972 LUMO: 0.60409 factor:1 | 1 (-0.09606) | -1 | -1 |
| G: -5717.87902 HOMO: -8.88180 LUMO: 1.02315 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.26774 HOMO: -7.38517 LUMO: 0.73743 factor:1 | 1 (-0.02302) | -1 | -1 |
| G: -5717.87902 HOMO: -8.88180 LUMO: 1.02315 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.32072 HOMO: -6.48992 LUMO: 1.08301 factor:1 | 1 (-0.07600) | -1 | -1 |
| G: -5717.87902 HOMO: -8.88180 LUMO: 1.02315 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.44616 HOMO: -7.18381 LUMO: 1.61908 factor:1 | 1 (-0.20145) | 1 | 1 |
| G: -5717.87902 HOMO: -8.88180 LUMO: 1.02315 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.31778 HOMO: -6.74842 LUMO: 0.57960 factor:1 | 1 (-0.07306) | -1 | -1 |
| G: -5717.87902 HOMO: -8.88180 LUMO: 1.02315 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.40401 HOMO: -6.67495 LUMO: 0.77280 factor:1 | 1 (-0.15930) | -1 | -1 |
| G: -5717.87902 HOMO: -8.88180 LUMO: 1.02315 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.64838 HOMO: -6.74570 LUMO: 0.77280 factor:1 | -1 (0.59634) | -1 | -1 |
| G: -5717.87902 HOMO: -8.88180 LUMO: 1.02315 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.86645 HOMO: -6.73754 LUMO: 0.86804 factor:1 | -1 (0.37827) | -1 | -1 |
| G: -5717.87902 HOMO: -8.88180 LUMO: 1.02315 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.26655 HOMO: -6.66135 LUMO: 0.94424 factor:1 | -1 (0.97817) | -1 | -1 |
| G: -5717.87902 HOMO: -8.88180 LUMO: 1.02315 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.39353 HOMO: -6.44638 LUMO: 1.00138 factor:1 | 1 (-0.14882) | -1 | -1 |
| G: -5717.87902 HOMO: -8.88180 LUMO: 1.02315 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.29576 HOMO: -6.65591 LUMO: 1.02043 factor:1 | 1 (-0.05105) | -1 | -1 |
| G: -5717.87902 HOMO: -8.88180 LUMO: 1.02315 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.95354 HOMO: -7.17564 LUMO: 0.50069 factor:1 | 1 (-0.70883) | -1 | -1 |
| G: -5717.87902 HOMO: -8.88180 LUMO: 1.02315 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.15859 HOMO: -6.59332 LUMO: 0.79457 factor:1 | -1 (0.08612) | -1 | -1 |
| G: -5717.87902 HOMO: -8.88180 LUMO: 1.02315 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.14616 HOMO: -6.76747 LUMO: 1.73881 factor:1 | -1 (0.09856) | -1 | -1 |
| G: -5717.87902 HOMO: -8.88180 LUMO: 1.02315 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.78884 HOMO: -7.00421 LUMO: 1.07485 factor:1 | -1 (0.45587) | -1 | -1 |
| G: -5717.87902 HOMO: -8.88180 LUMO: 1.02315 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.40583 HOMO: -6.94979 LUMO: 1.67894 factor:1 | 1 (-0.16112) | -1 | -1 |
| G: -5717.87902 HOMO: -8.88180 LUMO: 1.02315 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.32730 HOMO: -6.66135 LUMO: 0.47076 factor:1 | 1 (-0.08259) | -1 | -1 |
| G: -5717.87902 HOMO: -8.88180 LUMO: 1.02315 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.59857 HOMO: -6.74298 LUMO: 1.85037 factor:1 | 1 (-0.35386) | -1 | -1 |
| G: -5717.87902 HOMO: -8.88180 LUMO: 1.02315 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11983.22520 HOMO: -6.65318 LUMO: 0.95240 factor:1 | 1 (-0.98048) | -1 | -1 |
| G: -5717.87902 HOMO: -8.88180 LUMO: 1.02315 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.91112 HOMO: -6.63958 LUMO: 0.78097 factor:1 | 1 (-0.66641) | -1 | -1 |
| G: -5717.87902 HOMO: -8.88180 LUMO: 1.02315 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11983.03150 HOMO: -6.11712 LUMO: 0.40001 factor:1 | 1 (-0.78679) | -1 | -1 |
| G: -5717.87902 HOMO: -8.88180 LUMO: 1.02315 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.04445 HOMO: -7.08312 LUMO: 0.92519 factor:1 | -1 (1.20027) | -1 | -1 |
| G: -5717.87902 HOMO: -8.88180 LUMO: 1.02315 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.95639 HOMO: -6.96067 LUMO: 0.54695 factor:1 | -1 (1.28832) | -1 | -1 |
| G: -5717.87902 HOMO: -8.88180 LUMO: 1.02315 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.70737 HOMO: -6.74026 LUMO: 0.60137 factor:1 | -1 (0.53734) | -1 | -1 |
| G: -5717.87902 HOMO: -8.88180 LUMO: 1.02315 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.02227 HOMO: -6.74298 LUMO: 0.59593 factor:1 | -1 (1.22244) | -1 | -1 |
| G: -5717.87902 HOMO: -8.88180 LUMO: 1.02315 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.39964 HOMO: -6.93074 LUMO: 0.60681 factor:1 | -1 (0.84508) | -1 | -1 |
| G: -5717.87902 HOMO: -8.88180 LUMO: 1.02315 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.81456 HOMO: -6.41644 LUMO: 0.35919 factor:1 | -1 (0.43016) | -1 | -1 |
| G: -5717.87902 HOMO: -8.88180 LUMO: 1.02315 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.10796 HOMO: -6.41917 LUMO: 1.73064 factor:1 | -1 (1.13676) | -1 | -1 |
| G: -5717.87902 HOMO: -8.88180 LUMO: 1.02315 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.63088 HOMO: -4.64226 LUMO: -0.87893 factor:1 | -1 (0.61383) | -1 | -1 |
| G: -5717.87902 HOMO: -8.88180 LUMO: 1.02315 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.90197 HOMO: -6.59604 LUMO: 0.90342 factor:1 | -1 (1.34275) | -1 | -1 |
| G: -5717.87902 HOMO: -8.88180 LUMO: 1.02315 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.68443 HOMO: -6.79468 LUMO: 0.50069 factor:1 | -1 (0.56028) | -1 | -1 |
| G: -5717.87902 HOMO: -8.88180 LUMO: 1.02315 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.05599 HOMO: -7.04503 LUMO: 0.52518 factor:1 | -1 (1.18873) | -1 | -1 |
| G: -5717.87902 HOMO: -8.88180 LUMO: 1.02315 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.88833 HOMO: -6.69400 LUMO: 0.54423 factor:1 | -1 (0.35639) | -1 | -1 |
| G: -5717.87902 HOMO: -8.88180 LUMO: 1.02315 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.08829 HOMO: -6.51713 LUMO: 0.95240 factor:1 | -1 (1.15643) | -1 | -1 |
| G: -5717.87902 HOMO: -8.88180 LUMO: 1.02315 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.42554 HOMO: -6.88176 LUMO: 1.79323 factor:1 | -1 (0.81917) | -1 | -1 |
| G: -5717.87902 HOMO: -8.88180 LUMO: 1.02315 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.89679 HOMO: -6.71849 LUMO: 0.28844 factor:1 | -1 (0.34792) | -1 | -1 |
| G: -5717.87902 HOMO: -8.88180 LUMO: 1.02315 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.76043 HOMO: -6.94979 LUMO: 0.51974 factor:1 | -1 (0.48428) | -1 | -1 |
| G: -5717.87902 HOMO: -8.88180 LUMO: 1.02315 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.85233 HOMO: -6.76203 LUMO: 0.94151 factor:1 | -1 (0.39239) | -1 | -1 |
| G: -5717.87902 HOMO: -8.88180 LUMO: 1.02315 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.31614 HOMO: -6.91169 LUMO: 0.89525 factor:1 | 1 (-0.07143) | -1 | -1 |
| G: -5717.87902 HOMO: -8.88180 LUMO: 1.02315 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.24036 HOMO: -6.83006 LUMO: 0.89253 factor:1 | -1 (0.00435) | -1 | -1 |
| G: -5717.87902 HOMO: -8.88180 LUMO: 1.02315 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.20363 HOMO: -7.08857 LUMO: 0.60409 factor:1 | -1 (0.04109) | -1 | -1 |
| G: -5717.87902 HOMO: -8.88180 LUMO: 1.02315 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11983.62659 HOMO: -6.91713 LUMO: 1.76330 factor:1 | 1 (-1.38188) | -1 | -1 |
| G: -5717.87902 HOMO: -8.88180 LUMO: 1.02315 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11983.58303 HOMO: -6.47359 LUMO: 1.56193 factor:1 | 1 (-1.33831) | -1 | -1 |
| G: -5717.87902 HOMO: -6.91169 LUMO: -0.53879 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11983.61824 HOMO: -7.00149 LUMO: 1.47214 factor:1 | 1 (-1.37352) | -1 | -1 |
| G: -5717.87902 HOMO: -6.91169 LUMO: -0.53879 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11983.25069 HOMO: -7.03686 LUMO: 1.97283 factor:1 | 1 (-1.00598) | -1 | -1 |
| G: -5717.87902 HOMO: -6.91169 LUMO: -0.53879 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.60108 HOMO: -7.00965 LUMO: 1.64629 factor:1 | -1 (0.64363) | -1 | -1 |
| G: -5717.87902 HOMO: -6.91169 LUMO: -0.53879 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.24110 HOMO: -7.06952 LUMO: 1.67622 factor:1 | -1 (0.00362) | 1 | -1 |
| G: -5717.87902 HOMO: -6.91169 LUMO: -0.53879 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11979.80709 HOMO: -6.80557 LUMO: 1.70615 factor:1 | -1 (2.43762) | -1 | -1 |
| G: -5717.87902 HOMO: -6.91169 LUMO: -0.53879 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.27601 HOMO: -6.80829 LUMO: 1.71704 factor:1 | 1 (-0.03129) | -1 | -1 |
| G: -5717.87902 HOMO: -6.91169 LUMO: -0.53879 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.17837 HOMO: -7.26544 LUMO: 1.89935 factor:1 | -1 (0.06634) | 1 | -1 |
| G: -5717.87902 HOMO: -7.29809 LUMO: 2.83543 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.84222 HOMO: -7.00149 LUMO: 1.47214 factor:1 | 1 (-0.59751) | -1 | -1 |
| G: -5717.87902 HOMO: -7.29809 LUMO: 2.83543 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.96844 HOMO: -7.03686 LUMO: 1.97283 factor:1 | -1 (0.27628) | -1 | -1 |
| G: -5717.87902 HOMO: -7.29809 LUMO: 2.83543 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.34428 HOMO: -7.00965 LUMO: 1.64629 factor:1 | 1 (-0.09957) | -1 | -1 |
| G: -5717.87902 HOMO: -7.29809 LUMO: 2.83543 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.33133 HOMO: -7.06952 LUMO: 1.67622 factor:1 | 1 (-0.08661) | -1 | -1 |
| G: -5717.87902 HOMO: -7.29809 LUMO: 2.83543 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.69936 HOMO: -6.80557 LUMO: 1.70615 factor:1 | 1 (-0.45465) | -1 | -1 |
| G: -5717.87902 HOMO: -7.29809 LUMO: 2.83543 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.01410 HOMO: -6.80829 LUMO: 1.71704 factor:1 | -1 (0.23062) | -1 | -1 |
| G: -5717.87902 HOMO: -7.29809 LUMO: 2.83543 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.32772 HOMO: -7.26544 LUMO: 1.89935 factor:1 | -1 (0.91700) | -1 | -1 |
| G: -5717.87902 HOMO: -7.85865 LUMO: 2.83543 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.91815 HOMO: -7.00149 LUMO: 1.75241 factor:1 | -1 (0.32656) | -1 | -1 |
| G: -5717.87902 HOMO: -7.85865 LUMO: 2.83543 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.84490 HOMO: -6.91169 LUMO: 2.07079 factor:1 | -1 (0.39982) | -1 | -1 |
| G: -5717.87902 HOMO: -7.85865 LUMO: 2.83543 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.46813 HOMO: -7.11034 LUMO: 1.76330 factor:1 | -1 (0.77659) | -1 | -1 |
| G: -5717.87902 HOMO: -7.85865 LUMO: 2.83543 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.32777 HOMO: -6.87360 LUMO: 2.02725 factor:1 | -1 (0.91694) | -1 | -1 |
| G: -5717.87902 HOMO: -7.85865 LUMO: 2.83543 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.23424 HOMO: -7.08584 LUMO: 1.82044 factor:1 | -1 (0.01048) | -1 | -1 |
| G: -5717.87902 HOMO: -7.85865 LUMO: 2.83543 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.21448 HOMO: -6.90625 LUMO: 1.68166 factor:1 | -1 (0.03023) | -1 | -1 |
| G: -5717.87902 HOMO: -7.85865 LUMO: 2.83543 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.14776 HOMO: -6.71577 LUMO: 1.93201 factor:1 | -1 (0.09695) | -1 | -1 |
| G: -5717.87902 HOMO: -7.85865 LUMO: 2.83543 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.15124 HOMO: -6.99605 LUMO: 2.08439 factor:1 | -1 (0.09347) | -1 | -1 |
| G: -5717.87902 HOMO: -7.85865 LUMO: 2.83543 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.90947 HOMO: -7.02326 LUMO: 1.97010 factor:1 | -1 (0.33524) | -1 | -1 |
| G: -5717.87902 HOMO: -7.85865 LUMO: 2.83543 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.33721 HOMO: -6.99877 LUMO: 2.15514 factor:1 | 1 (-0.09249) | -1 | -1 |
| G: -5717.87902 HOMO: -7.85865 LUMO: 2.83543 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.31620 HOMO: -6.75387 LUMO: 1.95106 factor:1 | 1 (-0.07148) | -1 | -1 |
| G: -5717.87902 HOMO: -7.85865 LUMO: 2.83543 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.05798 HOMO: -7.10761 LUMO: 2.06262 factor:1 | -1 (2.18673) | -1 | -1 |
| G: -5717.87902 HOMO: -7.85865 LUMO: 2.83543 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11979.83379 HOMO: -7.03142 LUMO: 1.91568 factor:1 | -1 (2.41093) | -1 | -1 |
| G: -5717.87902 HOMO: -7.85865 LUMO: 2.83543 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.03261 HOMO: -6.98788 LUMO: 1.98371 factor:1 | -1 (1.21210) | -1 | -1 |
| G: -5717.87902 HOMO: -7.85865 LUMO: 2.83543 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.28121 HOMO: -6.94707 LUMO: 1.68438 factor:1 | -1 (0.96350) | -1 | -1 |
| G: -5717.87902 HOMO: -7.85865 LUMO: 2.83543 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.88871 HOMO: -6.88176 LUMO: 2.20684 factor:1 | -1 (0.35601) | -1 | -1 |
| G: -5717.87902 HOMO: -7.85865 LUMO: 2.83543 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.76577 HOMO: -6.73210 LUMO: 2.18780 factor:1 | -1 (0.47895) | -1 | -1 |
| G: -5717.87902 HOMO: -7.85865 LUMO: 2.83543 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.90763 HOMO: -6.83822 LUMO: 2.06807 factor:1 | -1 (1.33709) | -1 | -1 |
| G: -5717.87902 HOMO: -7.85865 LUMO: 2.83543 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.93928 HOMO: -6.78924 LUMO: 2.42181 factor:1 | -1 (1.30544) | -1 | -1 |
| G: -5717.87902 HOMO: -7.85865 LUMO: 2.83543 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.81458 HOMO: -6.94707 LUMO: 1.71704 factor:1 | -1 (0.43013) | -1 | -1 |
| G: -5717.87902 HOMO: -7.85865 LUMO: 2.83543 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.64138 HOMO: -6.85183 LUMO: 1.78779 factor:1 | -1 (0.60333) | -1 | -1 |
| G: -5717.87902 HOMO: -7.85865 LUMO: 2.83543 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.69145 HOMO: -6.98788 LUMO: 1.69799 factor:1 | -1 (0.55326) | -1 | -1 |
| G: -5717.87902 HOMO: -7.85865 LUMO: 2.83543 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.68992 HOMO: -6.79468 LUMO: 2.04358 factor:1 | 1 (-0.44521) | -1 | -1 |
| G: -5717.87902 HOMO: -7.85865 LUMO: 2.83543 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.91232 HOMO: -6.90081 LUMO: 1.97283 factor:1 | 1 (-0.66760) | -1 | -1 |
| G: -5717.87902 HOMO: -7.85865 LUMO: 2.83543 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.10942 HOMO: -6.79468 LUMO: 2.00820 factor:1 | -1 (0.13530) | -1 | -1 |
| G: -5717.87902 HOMO: -7.85865 LUMO: 2.83543 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.10528 HOMO: -7.06408 LUMO: 2.29936 factor:1 | -1 (0.13943) | -1 | -1 |
| G: -5717.87902 HOMO: -7.85865 LUMO: 2.83543 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.12670 HOMO: -6.78924 LUMO: 2.13337 factor:1 | -1 (0.11802) | -1 | -1 |
| G: -5717.87902 HOMO: -7.85865 LUMO: 2.83543 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.20532 HOMO: -6.79468 LUMO: 2.35106 factor:1 | -1 (1.03939) | -1 | -1 |
| G: -5717.87902 HOMO: -7.85865 LUMO: 2.83543 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.22957 HOMO: -6.82734 LUMO: 2.16603 factor:1 | -1 (1.01515) | -1 | -1 |
| G: -5717.87902 HOMO: -7.85865 LUMO: 2.83543 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.80365 HOMO: -6.79740 LUMO: 2.36739 factor:1 | -1 (0.44107) | -1 | -1 |
| G: -5717.87902 HOMO: -7.85865 LUMO: 2.83543 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.20712 HOMO: -7.14027 LUMO: 2.10888 factor:1 | -1 (1.03760) | -1 | -1 |
| G: -5717.87902 HOMO: -6.61509 LUMO: -0.23674 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.97222 HOMO: -6.96067 LUMO: 1.59731 factor:1 | -1 (0.27249) | -1 | -1 |
| G: -5717.87902 HOMO: -6.61509 LUMO: -0.23674 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.09429 HOMO: -6.91169 LUMO: 1.37145 factor:1 | -1 (0.15042) | -1 | -1 |
| G: -5717.87902 HOMO: -6.61509 LUMO: -0.23674 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.20402 HOMO: -6.94707 LUMO: 1.73064 factor:1 | -1 (1.04070) | -1 | -1 |
| G: -5717.87902 HOMO: -6.61509 LUMO: -0.23674 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.24799 HOMO: -7.02326 LUMO: 1.41227 factor:1 | -1 (0.99673) | -1 | -1 |
| G: -5717.87902 HOMO: -6.61509 LUMO: -0.23674 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.45441 HOMO: -6.72121 LUMO: 1.43132 factor:1 | -1 (0.79030) | -1 | -1 |
| G: -5717.87902 HOMO: -6.61509 LUMO: -0.23674 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.84090 HOMO: -6.51168 LUMO: 1.72520 factor:1 | -1 (0.40382) | -1 | -1 |
| G: -5717.87902 HOMO: -6.61509 LUMO: -0.23674 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.20804 HOMO: -6.98516 LUMO: 1.92929 factor:1 | -1 (1.03667) | -1 | -1 |
| G: -5717.87902 HOMO: -6.61509 LUMO: -0.23674 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.53135 HOMO: -6.92802 LUMO: 2.07895 factor:1 | -1 (1.71336) | -1 | -1 |
| G: -5717.87902 HOMO: -6.61509 LUMO: -0.23674 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.83669 HOMO: -7.02326 LUMO: 1.86398 factor:1 | -1 (1.40803) | -1 | -1 |
| G: -5717.87902 HOMO: -6.61509 LUMO: -0.23674 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.07894 HOMO: -6.82462 LUMO: 1.86670 factor:1 | -1 (0.16577) | -1 | -1 |
| G: -5717.87902 HOMO: -6.61509 LUMO: -0.23674 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.85535 HOMO: -6.83278 LUMO: 1.71160 factor:1 | -1 (0.38937) | -1 | -1 |
| G: -5717.87902 HOMO: -6.61509 LUMO: -0.23674 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.16701 HOMO: -6.62869 LUMO: 1.69527 factor:1 | -1 (1.07771) | -1 | -1 |
| G: -5717.87902 HOMO: -6.61509 LUMO: -0.23674 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.05569 HOMO: -6.84094 LUMO: 1.27349 factor:1 | -1 (1.18903) | -1 | -1 |
| G: -5717.87902 HOMO: -6.61509 LUMO: -0.23674 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.59764 HOMO: -7.07768 LUMO: 1.27621 factor:1 | -1 (1.64708) | 1 | -1 |
| G: -5717.87902 HOMO: -6.61509 LUMO: -0.23674 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11983.26721 HOMO: -7.06135 LUMO: 1.55105 factor:1 | 1 (-1.02250) | 1 | -1 |
| G: -5717.87902 HOMO: -6.61509 LUMO: -0.23674 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.51599 HOMO: -6.94162 LUMO: 1.64629 factor:1 | 1 (-0.27127) | -1 | -1 |
| G: -5717.87902 HOMO: -6.61509 LUMO: -0.23674 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11983.22079 HOMO: -7.07224 LUMO: 1.65445 factor:1 | 1 (-0.97607) | 1 | -1 |
| G: -5717.87902 HOMO: -6.61509 LUMO: -0.23674 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11983.22125 HOMO: -6.68584 LUMO: 1.91296 factor:1 | 1 (-0.97654) | -1 | -1 |
| G: -5717.87902 HOMO: -6.61509 LUMO: -0.23674 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.53743 HOMO: -7.09129 LUMO: 1.73609 factor:1 | 1 (-0.29271) | 1 | -1 |
| G: -5717.87902 HOMO: -6.61509 LUMO: -0.23674 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.97954 HOMO: -7.01237 LUMO: 2.01092 factor:1 | -1 (0.26517) | -1 | -1 |
| G: -5717.87902 HOMO: -6.61509 LUMO: -0.23674 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.96212 HOMO: -6.93618 LUMO: 1.63540 factor:1 | -1 (0.28259) | -1 | -1 |
| G: -5717.87902 HOMO: -6.61509 LUMO: -0.23674 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.11261 HOMO: -6.98516 LUMO: 1.64629 factor:1 | -1 (1.13210) | -1 | -1 |
| G: -5717.87902 HOMO: -6.61509 LUMO: -0.23674 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.51686 HOMO: -6.80285 LUMO: 1.95106 factor:1 | -1 (0.72785) | -1 | -1 |
| G: -5717.87902 HOMO: -6.61509 LUMO: -0.23674 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.69772 HOMO: -6.76747 LUMO: 1.88303 factor:1 | -1 (1.54699) | -1 | -1 |
| G: -5717.87902 HOMO: -6.61509 LUMO: -0.23674 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.11125 HOMO: -6.64230 LUMO: 1.90480 factor:1 | -1 (1.13346) | -1 | -1 |
| G: -5717.87902 HOMO: -6.61509 LUMO: -0.23674 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.99669 HOMO: -6.93618 LUMO: 2.19324 factor:1 | -1 (1.24802) | -1 | -1 |
| G: -5717.87902 HOMO: -6.61509 LUMO: -0.23674 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11983.21692 HOMO: -6.95523 LUMO: 1.80684 factor:1 | 1 (-0.97221) | -1 | -1 |
| G: -5717.87902 HOMO: -6.61509 LUMO: -0.23674 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11983.18732 HOMO: -6.66135 LUMO: 1.72792 factor:1 | 1 (-0.94260) | -1 | -1 |
| G: -5717.87902 HOMO: -6.61509 LUMO: -0.23674 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.43484 HOMO: -6.36202 LUMO: 1.89391 factor:1 | 1 (-0.19013) | -1 | -1 |
| G: -5717.87902 HOMO: -6.61509 LUMO: -0.23674 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.37035 HOMO: -7.03959 LUMO: 2.06262 factor:1 | 1 (-0.12563) | -1 | -1 |
| G: -5717.87902 HOMO: -6.61509 LUMO: -0.23674 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11983.11692 HOMO: -7.08584 LUMO: 2.01092 factor:1 | 1 (-0.87221) | 1 | -1 |
| G: -5717.87902 HOMO: -6.80285 LUMO: -0.55783 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.86164 HOMO: -6.96067 LUMO: 1.59731 factor:1 | -1 (1.38307) | -1 | -1 |
| G: -5717.87902 HOMO: -6.80285 LUMO: -0.55783 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.73241 HOMO: -6.91169 LUMO: 1.37145 factor:1 | -1 (0.51231) | -1 | -1 |
| G: -5717.87902 HOMO: -6.80285 LUMO: -0.55783 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.97914 HOMO: -6.94707 LUMO: 1.73064 factor:1 | -1 (1.26557) | -1 | -1 |
| G: -5717.87902 HOMO: -6.80285 LUMO: -0.55783 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11983.18261 HOMO: -7.02326 LUMO: 1.41227 factor:1 | 1 (-0.93789) | -1 | -1 |
| G: -5717.87902 HOMO: -6.80285 LUMO: -0.55783 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11983.21145 HOMO: -6.72121 LUMO: 1.43132 factor:1 | 1 (-0.96674) | -1 | -1 |
| G: -5717.87902 HOMO: -6.80285 LUMO: -0.55783 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.35974 HOMO: -6.51168 LUMO: 1.72520 factor:1 | 1 (-0.11502) | -1 | -1 |
| G: -5717.87902 HOMO: -6.80285 LUMO: -0.55783 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.23476 HOMO: -6.98516 LUMO: 1.92929 factor:1 | -1 (0.00996) | -1 | -1 |
| G: -5717.87902 HOMO: -6.80285 LUMO: -0.55783 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.86739 HOMO: -6.92802 LUMO: 2.07895 factor:1 | 1 (-0.62268) | -1 | -1 |
| G: -5717.87902 HOMO: -6.80285 LUMO: -0.55783 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.89505 HOMO: -7.02326 LUMO: 1.86398 factor:1 | -1 (0.34967) | -1 | -1 |
| G: -5717.87902 HOMO: -6.80285 LUMO: -0.55783 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.05340 HOMO: -6.82462 LUMO: 1.86670 factor:1 | -1 (1.19131) | -1 | -1 |
| G: -5717.87902 HOMO: -6.80285 LUMO: -0.55783 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.45545 HOMO: -6.83278 LUMO: 1.71160 factor:1 | -1 (0.78927) | -1 | -1 |
| G: -5717.87902 HOMO: -6.80285 LUMO: -0.55783 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.87606 HOMO: -6.62869 LUMO: 1.69527 factor:1 | -1 (1.36865) | -1 | -1 |
| G: -5717.87902 HOMO: -6.80285 LUMO: -0.55783 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.09052 HOMO: -6.84094 LUMO: 1.27349 factor:1 | -1 (1.15420) | -1 | -1 |
| G: -5717.87902 HOMO: -6.80285 LUMO: -0.55783 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.98212 HOMO: -7.07768 LUMO: 1.27621 factor:1 | -1 (0.26259) | 1 | -1 |
| G: -5717.87902 HOMO: -6.80285 LUMO: -0.55783 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.05272 HOMO: -7.06135 LUMO: 1.55105 factor:1 | -1 (1.19199) | 1 | -1 |
| G: -5717.87902 HOMO: -6.80285 LUMO: -0.55783 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.94364 HOMO: -6.94162 LUMO: 1.64629 factor:1 | 1 (-0.69892) | -1 | -1 |
| G: -5717.87902 HOMO: -6.80285 LUMO: -0.55783 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.13369 HOMO: -7.07224 LUMO: 1.65445 factor:1 | -1 (0.11102) | 1 | -1 |
| G: -5717.87902 HOMO: -6.80285 LUMO: -0.55783 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.85839 HOMO: -6.68584 LUMO: 1.91296 factor:1 | 1 (-0.61367) | -1 | -1 |
| G: -5717.87902 HOMO: -6.80285 LUMO: -0.55783 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.01576 HOMO: -7.09129 LUMO: 1.73609 factor:1 | -1 (0.22896) | 1 | -1 |
| G: -5717.87902 HOMO: -6.80285 LUMO: -0.55783 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.64974 HOMO: -7.01237 LUMO: 2.01092 factor:1 | -1 (0.59498) | -1 | -1 |
| G: -5717.87902 HOMO: -6.80285 LUMO: -0.55783 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.86315 HOMO: -6.93618 LUMO: 1.63540 factor:1 | 1 (-0.61843) | -1 | -1 |
| G: -5717.87902 HOMO: -6.80285 LUMO: -0.55783 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.97467 HOMO: -6.98516 LUMO: 1.64629 factor:1 | -1 (0.27005) | -1 | -1 |
| G: -5717.87902 HOMO: -6.80285 LUMO: -0.55783 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.71474 HOMO: -6.80285 LUMO: 1.95106 factor:1 | 1 (-0.47002) | -1 | -1 |
| G: -5717.87902 HOMO: -6.80285 LUMO: -0.55783 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11979.55400 HOMO: -6.76747 LUMO: 1.88303 factor:1 | -1 (2.69072) | -1 | -1 |
| G: -5717.87902 HOMO: -6.80285 LUMO: -0.55783 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.76175 HOMO: -6.64230 LUMO: 1.90480 factor:1 | -1 (1.48297) | -1 | -1 |
| G: -5717.87902 HOMO: -6.80285 LUMO: -0.55783 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.50044 HOMO: -6.93618 LUMO: 2.19324 factor:1 | -1 (1.74428) | -1 | -1 |
| G: -5717.87902 HOMO: -6.80285 LUMO: -0.55783 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.61963 HOMO: -6.95523 LUMO: 1.80684 factor:1 | 1 (-0.37492) | -1 | -1 |
| G: -5717.87902 HOMO: -6.80285 LUMO: -0.55783 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.12343 HOMO: -6.66135 LUMO: 1.72792 factor:1 | -1 (0.12128) | -1 | -1 |
| G: -5717.87902 HOMO: -6.80285 LUMO: -0.55783 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.69836 HOMO: -6.36202 LUMO: 1.89391 factor:1 | 1 (-0.45364) | -1 | -1 |
| G: -5717.87902 HOMO: -6.80285 LUMO: -0.55783 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.28771 HOMO: -7.03959 LUMO: 2.06262 factor:1 | 1 (-0.04299) | -1 | -1 |
| G: -5717.87902 HOMO: -6.80285 LUMO: -0.55783 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.42878 HOMO: -7.08584 LUMO: 2.01092 factor:1 | -1 (0.81593) | 1 | -1 |
| G: -5717.87902 HOMO: -7.16476 LUMO: 2.86264 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.18502 HOMO: -6.96067 LUMO: 1.59731 factor:1 | -1 (1.05969) | -1 | -1 |
| G: -5717.87902 HOMO: -7.16476 LUMO: 2.86264 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.33984 HOMO: -6.91169 LUMO: 1.37145 factor:1 | -1 (1.90488) | -1 | -1 |
| G: -5717.87902 HOMO: -7.16476 LUMO: 2.86264 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.14395 HOMO: -6.94707 LUMO: 1.73064 factor:1 | -1 (0.10076) | -1 | -1 |
| G: -5717.87902 HOMO: -7.16476 LUMO: 2.86264 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.14391 HOMO: -7.02326 LUMO: 1.41227 factor:1 | -1 (1.10081) | -1 | -1 |
| G: -5717.87902 HOMO: -7.16476 LUMO: 2.86264 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.83595 HOMO: -6.72121 LUMO: 1.43132 factor:1 | -1 (0.40877) | -1 | -1 |
| G: -5717.87902 HOMO: -7.16476 LUMO: 2.86264 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.23805 HOMO: -6.51168 LUMO: 1.72520 factor:1 | -1 (0.00667) | -1 | -1 |
| G: -5717.87902 HOMO: -7.16476 LUMO: 2.86264 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.30366 HOMO: -6.98516 LUMO: 1.92929 factor:1 | -1 (0.94105) | -1 | -1 |
| G: -5717.87902 HOMO: -7.16476 LUMO: 2.86264 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.05132 HOMO: -6.92802 LUMO: 2.07895 factor:1 | -1 (0.19339) | -1 | -1 |
| G: -5717.87902 HOMO: -7.16476 LUMO: 2.86264 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.14976 HOMO: -7.02326 LUMO: 1.86398 factor:1 | -1 (1.09496) | -1 | -1 |
| G: -5717.87902 HOMO: -7.16476 LUMO: 2.86264 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.91545 HOMO: -6.82462 LUMO: 1.86670 factor:1 | 1 (-0.67073) | -1 | -1 |
| G: -5717.87902 HOMO: -7.16476 LUMO: 2.86264 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11983.31804 HOMO: -6.83278 LUMO: 1.71160 factor:1 | 1 (-1.07333) | -1 | -1 |
| G: -5717.87902 HOMO: -7.16476 LUMO: 2.86264 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.10254 HOMO: -6.62869 LUMO: 1.69527 factor:1 | -1 (0.14218) | -1 | -1 |
| G: -5717.87902 HOMO: -7.16476 LUMO: 2.86264 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.30828 HOMO: -6.84094 LUMO: 1.27349 factor:1 | 1 (-0.06357) | -1 | -1 |
| G: -5717.87902 HOMO: -7.16476 LUMO: 2.86264 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.65275 HOMO: -7.07768 LUMO: 1.27621 factor:1 | 1 (-0.40803) | -1 | -1 |
| G: -5717.87902 HOMO: -7.16476 LUMO: 2.86264 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.34401 HOMO: -7.06135 LUMO: 1.55105 factor:1 | 1 (-0.09929) | -1 | -1 |
| G: -5717.87902 HOMO: -7.16476 LUMO: 2.86264 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11983.15521 HOMO: -6.94162 LUMO: 1.64629 factor:1 | 1 (-0.91049) | -1 | -1 |
| G: -5717.87902 HOMO: -7.16476 LUMO: 2.86264 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.82962 HOMO: -7.07224 LUMO: 1.65445 factor:1 | 1 (-0.58491) | -1 | -1 |
| G: -5717.87902 HOMO: -7.16476 LUMO: 2.86264 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.47463 HOMO: -6.68584 LUMO: 1.91296 factor:1 | -1 (0.77008) | -1 | -1 |
| G: -5717.87902 HOMO: -7.16476 LUMO: 2.86264 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.39918 HOMO: -7.09129 LUMO: 1.73609 factor:1 | -1 (1.84553) | -1 | -1 |
| G: -5717.87902 HOMO: -7.16476 LUMO: 2.86264 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.34585 HOMO: -7.01237 LUMO: 2.01092 factor:1 | -1 (1.89886) | -1 | -1 |
| G: -5717.87902 HOMO: -7.16476 LUMO: 2.86264 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.21040 HOMO: -6.93618 LUMO: 1.63540 factor:1 | -1 (0.03431) | -1 | -1 |
| G: -5717.87902 HOMO: -7.16476 LUMO: 2.86264 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.35917 HOMO: -6.98516 LUMO: 1.64629 factor:1 | -1 (0.88554) | -1 | -1 |
| G: -5717.87902 HOMO: -7.16476 LUMO: 2.86264 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.24926 HOMO: -6.80285 LUMO: 1.95106 factor:1 | 1 (-0.00454) | -1 | -1 |
| G: -5717.87902 HOMO: -7.16476 LUMO: 2.86264 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.48342 HOMO: -6.76747 LUMO: 1.88303 factor:1 | -1 (0.76129) | -1 | -1 |
| G: -5717.87902 HOMO: -7.16476 LUMO: 2.86264 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.88465 HOMO: -6.64230 LUMO: 1.90480 factor:1 | -1 (0.36006) | -1 | -1 |
| G: -5717.87902 HOMO: -7.16476 LUMO: 2.86264 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.33440 HOMO: -6.93618 LUMO: 2.19324 factor:1 | 1 (-0.08969) | -1 | -1 |
| G: -5717.87902 HOMO: -7.16476 LUMO: 2.86264 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11983.50096 HOMO: -6.95523 LUMO: 1.80684 factor:1 | 1 (-1.25624) | -1 | -1 |
| G: -5717.87902 HOMO: -7.16476 LUMO: 2.86264 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.48741 HOMO: -6.66135 LUMO: 1.72792 factor:1 | 1 (-0.24270) | -1 | -1 |
| G: -5717.87902 HOMO: -7.16476 LUMO: 2.86264 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11983.41268 HOMO: -6.36202 LUMO: 1.89391 factor:1 | 1 (-1.16797) | -1 | -1 |
| G: -5717.87902 HOMO: -7.16476 LUMO: 2.86264 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.80342 HOMO: -7.03959 LUMO: 2.06262 factor:1 | 1 (-0.55870) | -1 | -1 |
| G: -5717.87902 HOMO: -7.16476 LUMO: 2.86264 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.19413 HOMO: -7.08584 LUMO: 2.01092 factor:1 | -1 (0.05059) | -1 | -1 |
| G: -5717.87902 HOMO: -6.50352 LUMO: 2.10888 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.91186 HOMO: -6.96067 LUMO: 1.59731 factor:1 | 1 (-0.66714) | 1 | 1 |
| G: -5717.87902 HOMO: -6.50352 LUMO: 2.10888 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.48714 HOMO: -6.91169 LUMO: 1.37145 factor:1 | 1 (-0.24243) | -1 | -1 |
| G: -5717.87902 HOMO: -6.50352 LUMO: 2.10888 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11983.20430 HOMO: -6.94707 LUMO: 1.73064 factor:1 | 1 (-0.95958) | 1 | 1 |
| G: -5717.87902 HOMO: -6.50352 LUMO: 2.10888 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.40970 HOMO: -7.02326 LUMO: 1.41227 factor:1 | 1 (-0.16498) | -1 | -1 |
| G: -5717.87902 HOMO: -6.50352 LUMO: 2.10888 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.32942 HOMO: -6.72121 LUMO: 1.43132 factor:1 | 1 (-0.08471) | -1 | -1 |
| G: -5717.87902 HOMO: -6.50352 LUMO: 2.10888 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.97590 HOMO: -6.51168 LUMO: 1.72520 factor:1 | -1 (1.26881) | 1 | 1 |
| G: -5717.87902 HOMO: -6.50352 LUMO: 2.10888 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.11610 HOMO: -6.98516 LUMO: 1.92929 factor:1 | -1 (1.12862) | 1 | 1 |
| G: -5717.87902 HOMO: -6.50352 LUMO: 2.10888 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.85676 HOMO: -6.92802 LUMO: 2.07895 factor:1 | -1 (0.38795) | 1 | 1 |
| G: -5717.87902 HOMO: -6.50352 LUMO: 2.10888 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.99497 HOMO: -7.02326 LUMO: 1.86398 factor:1 | -1 (0.24975) | 1 | 1 |
| G: -5717.87902 HOMO: -6.50352 LUMO: 2.10888 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.87799 HOMO: -6.82462 LUMO: 1.86670 factor:1 | -1 (0.36673) | 1 | 1 |
| G: -5717.87902 HOMO: -6.50352 LUMO: 2.10888 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.19143 HOMO: -6.83278 LUMO: 1.71160 factor:1 | -1 (0.05328) | 1 | 1 |
| G: -5717.87902 HOMO: -6.50352 LUMO: 2.10888 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.66078 HOMO: -6.62869 LUMO: 1.69527 factor:1 | 1 (-0.41606) | 1 | 1 |
| G: -5717.87902 HOMO: -6.50352 LUMO: 2.10888 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.94437 HOMO: -6.84094 LUMO: 1.27349 factor:1 | 1 (-0.69966) | -1 | -1 |
| G: -5717.87902 HOMO: -6.50352 LUMO: 2.10888 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.10313 HOMO: -7.07768 LUMO: 1.27621 factor:1 | -1 (0.14158) | -1 | -1 |
| G: -5717.87902 HOMO: -6.50352 LUMO: 2.10888 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11983.18266 HOMO: -7.06135 LUMO: 1.55105 factor:1 | 1 (-0.93795) | -1 | -1 |
| G: -5717.87902 HOMO: -6.50352 LUMO: 2.10888 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.34613 HOMO: -6.94162 LUMO: 1.64629 factor:1 | 1 (-0.10142) | 1 | 1 |
| G: -5717.87902 HOMO: -6.50352 LUMO: 2.10888 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.23067 HOMO: -7.07224 LUMO: 1.65445 factor:1 | -1 (0.01404) | 1 | 1 |
| G: -5717.87902 HOMO: -6.50352 LUMO: 2.10888 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.87020 HOMO: -6.68584 LUMO: 1.91296 factor:1 | -1 (0.37451) | 1 | 1 |
| G: -5717.87902 HOMO: -6.50352 LUMO: 2.10888 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.23053 HOMO: -7.09129 LUMO: 1.73609 factor:1 | -1 (2.01419) | 1 | 1 |
| G: -5717.87902 HOMO: -6.50352 LUMO: 2.10888 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.91873 HOMO: -7.01237 LUMO: 2.01092 factor:1 | -1 (1.32598) | 1 | 1 |
| G: -5717.87902 HOMO: -6.50352 LUMO: 2.10888 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.98747 HOMO: -6.93618 LUMO: 1.63540 factor:1 | -1 (1.25725) | 1 | 1 |
| G: -5717.87902 HOMO: -6.50352 LUMO: 2.10888 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.02002 HOMO: -6.98516 LUMO: 1.64629 factor:1 | -1 (2.22469) | 1 | 1 |
| G: -5717.87902 HOMO: -6.50352 LUMO: 2.10888 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.23739 HOMO: -6.80285 LUMO: 1.95106 factor:1 | -1 (0.00732) | 1 | 1 |
| G: -5717.87902 HOMO: -6.50352 LUMO: 2.10888 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.56652 HOMO: -6.76747 LUMO: 1.88303 factor:1 | 1 (-0.32180) | 1 | 1 |
| G: -5717.87902 HOMO: -6.50352 LUMO: 2.10888 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.75551 HOMO: -6.64230 LUMO: 1.90480 factor:1 | -1 (0.48921) | 1 | 1 |
| G: -5717.87902 HOMO: -6.50352 LUMO: 2.10888 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.15837 HOMO: -6.93618 LUMO: 2.19324 factor:1 | -1 (0.08634) | 1 | 1 |
| G: -5717.87902 HOMO: -6.50352 LUMO: 2.10888 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.84795 HOMO: -6.95523 LUMO: 1.80684 factor:1 | -1 (0.39677) | 1 | 1 |
| G: -5717.87902 HOMO: -6.50352 LUMO: 2.10888 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.90439 HOMO: -6.66135 LUMO: 1.72792 factor:1 | -1 (1.34032) | 1 | 1 |
| G: -5717.87902 HOMO: -6.50352 LUMO: 2.10888 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.22848 HOMO: -6.36202 LUMO: 1.89391 factor:1 | -1 (1.01624) | -1 | -1 |
| G: -5717.87902 HOMO: -6.50352 LUMO: 2.10888 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.01925 HOMO: -7.03959 LUMO: 2.06262 factor:1 | -1 (1.22546) | 1 | 1 |
| G: -5717.87902 HOMO: -6.50352 LUMO: 2.10888 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.13911 HOMO: -7.08584 LUMO: 2.01092 factor:1 | -1 (0.10561) | 1 | 1 |
| G: -5717.87902 HOMO: -6.59604 LUMO: 2.33746 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.33213 HOMO: -6.96067 LUMO: 1.59731 factor:1 | -1 (0.91259) | 1 | 1 |
| G: -5717.87902 HOMO: -6.59604 LUMO: 2.33746 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.93345 HOMO: -6.91169 LUMO: 1.37145 factor:1 | -1 (1.31126) | -1 | -1 |
| G: -5717.87902 HOMO: -6.59604 LUMO: 2.33746 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.03988 HOMO: -6.94707 LUMO: 1.73064 factor:1 | -1 (1.20484) | 1 | 1 |
| G: -5717.87902 HOMO: -6.59604 LUMO: 2.33746 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.89857 HOMO: -7.02326 LUMO: 1.41227 factor:1 | -1 (1.34615) | -1 | -1 |
| G: -5717.87902 HOMO: -6.59604 LUMO: 2.33746 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.04945 HOMO: -6.72121 LUMO: 1.43132 factor:1 | -1 (0.19527) | -1 | -1 |
| G: -5717.87902 HOMO: -6.59604 LUMO: 2.33746 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.16772 HOMO: -6.51168 LUMO: 1.72520 factor:1 | -1 (1.07700) | -1 | -1 |
| G: -5717.87902 HOMO: -6.59604 LUMO: 2.33746 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.91530 HOMO: -6.98516 LUMO: 1.92929 factor:1 | -1 (1.32941) | 1 | 1 |
| G: -5717.87902 HOMO: -6.59604 LUMO: 2.33746 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.07951 HOMO: -6.92802 LUMO: 2.07895 factor:1 | -1 (0.16520) | 1 | 1 |
| G: -5717.87902 HOMO: -6.59604 LUMO: 2.33746 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.11169 HOMO: -7.02326 LUMO: 1.86398 factor:1 | -1 (1.13303) | 1 | 1 |
| G: -5717.87902 HOMO: -6.59604 LUMO: 2.33746 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.76381 HOMO: -6.82462 LUMO: 1.86670 factor:1 | -1 (0.48091) | 1 | 1 |
| G: -5717.87902 HOMO: -6.59604 LUMO: 2.33746 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.67865 HOMO: -6.83278 LUMO: 1.71160 factor:1 | -1 (1.56607) | 1 | 1 |
| G: -5717.87902 HOMO: -6.59604 LUMO: 2.33746 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.56988 HOMO: -6.62869 LUMO: 1.69527 factor:1 | -1 (1.67483) | 1 | 1 |
| G: -5717.87902 HOMO: -6.59604 LUMO: 2.33746 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.82227 HOMO: -6.84094 LUMO: 1.27349 factor:1 | -1 (1.42245) | -1 | -1 |
| G: -5717.87902 HOMO: -6.59604 LUMO: 2.33746 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.76356 HOMO: -7.07768 LUMO: 1.27621 factor:1 | -1 (0.48115) | -1 | -1 |
| G: -5717.87902 HOMO: -6.59604 LUMO: 2.33746 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.67567 HOMO: -7.06135 LUMO: 1.55105 factor:1 | -1 (0.56904) | -1 | -1 |
| G: -5717.87902 HOMO: -6.59604 LUMO: 2.33746 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.49193 HOMO: -6.94162 LUMO: 1.64629 factor:1 | 1 (-0.24722) | 1 | 1 |
| G: -5717.87902 HOMO: -6.59604 LUMO: 2.33746 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.87818 HOMO: -7.07224 LUMO: 1.65445 factor:1 | -1 (0.36654) | 1 | 1 |
| G: -5717.87902 HOMO: -6.59604 LUMO: 2.33746 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.58193 HOMO: -6.68584 LUMO: 1.91296 factor:1 | -1 (0.66279) | 1 | 1 |
| G: -5717.87902 HOMO: -6.59604 LUMO: 2.33746 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.51027 HOMO: -7.09129 LUMO: 1.73609 factor:1 | 1 (-0.26556) | 1 | 1 |
| G: -5717.87902 HOMO: -6.59604 LUMO: 2.33746 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11983.15937 HOMO: -7.01237 LUMO: 2.01092 factor:1 | 1 (-0.91466) | 1 | 1 |
| G: -5717.87902 HOMO: -6.59604 LUMO: 2.33746 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.46986 HOMO: -6.93618 LUMO: 1.63540 factor:1 | 1 (-0.22515) | 1 | 1 |
| G: -5717.87902 HOMO: -6.59604 LUMO: 2.33746 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.99442 HOMO: -6.98516 LUMO: 1.64629 factor:1 | 1 (-0.74970) | 1 | 1 |
| G: -5717.87902 HOMO: -6.59604 LUMO: 2.33746 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.30687 HOMO: -6.80285 LUMO: 1.95106 factor:1 | 1 (-0.06215) | 1 | 1 |
| G: -5717.87902 HOMO: -6.59604 LUMO: 2.33746 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.41778 HOMO: -6.76747 LUMO: 1.88303 factor:1 | 1 (-0.17306) | 1 | 1 |
| G: -5717.87902 HOMO: -6.59604 LUMO: 2.33746 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11983.17616 HOMO: -6.64230 LUMO: 1.90480 factor:1 | 1 (-0.93145) | 1 | 1 |
| G: -5717.87902 HOMO: -6.59604 LUMO: 2.33746 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11983.42188 HOMO: -6.93618 LUMO: 2.19324 factor:1 | 1 (-1.17716) | 1 | 1 |
| G: -5717.87902 HOMO: -6.59604 LUMO: 2.33746 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.53786 HOMO: -6.95523 LUMO: 1.80684 factor:1 | 1 (-0.29315) | 1 | 1 |
| G: -5717.87902 HOMO: -6.59604 LUMO: 2.33746 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.60565 HOMO: -6.66135 LUMO: 1.72792 factor:1 | 1 (-0.36093) | 1 | 1 |
| G: -5717.87902 HOMO: -6.59604 LUMO: 2.33746 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.50001 HOMO: -6.36202 LUMO: 1.89391 factor:1 | 1 (-0.25530) | -1 | -1 |
| G: -5717.87902 HOMO: -6.59604 LUMO: 2.33746 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.41197 HOMO: -7.03959 LUMO: 2.06262 factor:1 | -1 (1.83274) | 1 | 1 |
| G: -5717.87902 HOMO: -6.59604 LUMO: 2.33746 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.54894 HOMO: -7.08584 LUMO: 2.01092 factor:1 | 1 (-0.30422) | 1 | 1 |
| G: -5717.87902 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.16841 HOMO: -7.06135 LUMO: 0.75376 factor:1 | -1 (0.07630) | 1 | -1 |
| G: -5717.87902 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.26625 HOMO: -5.10213 LUMO: 0.77825 factor:1 | -1 (0.97847) | -1 | -1 |
| G: -5717.87902 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.61645 HOMO: -5.84228 LUMO: 0.50341 factor:1 | 1 (-0.37173) | -1 | -1 |
| G: -5717.87902 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.59185 HOMO: -5.39874 LUMO: 0.68028 factor:1 | 1 (-0.34714) | -1 | -1 |
| G: -5717.87902 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.38218 HOMO: -5.16744 LUMO: 1.14832 factor:1 | -1 (1.86254) | -1 | -1 |
| G: -5717.87902 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.44733 HOMO: -5.80963 LUMO: 0.35647 factor:1 | 1 (-0.20262) | -1 | -1 |
| G: -5717.87902 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.06987 HOMO: -5.02322 LUMO: 1.07213 factor:1 | -1 (2.17484) | -1 | -1 |
| G: -5717.87902 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11979.88524 HOMO: -5.80963 LUMO: 0.56328 factor:1 | -1 (2.35947) | -1 | -1 |
| G: -5717.87902 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.31586 HOMO: -5.45316 LUMO: 0.78369 factor:1 | -1 (1.92885) | -1 | -1 |
| G: -5717.87902 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.92588 HOMO: -5.25452 LUMO: 0.82178 factor:1 | -1 (0.31884) | -1 | -1 |
| G: -5717.87902 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.18714 HOMO: -5.21370 LUMO: 1.03947 factor:1 | -1 (1.05757) | -1 | -1 |
| G: -5717.87902 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11979.97948 HOMO: -6.04365 LUMO: 0.31837 factor:1 | -1 (2.26524) | -1 | -1 |
| G: -5717.87902 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.39869 HOMO: -5.86405 LUMO: 0.55511 factor:1 | -1 (1.84602) | -1 | -1 |
| G: -5717.87902 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.71898 HOMO: -5.64908 LUMO: 0.71022 factor:1 | 1 (-0.47427) | -1 | -1 |
| G: -5717.87902 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.23348 HOMO: -5.94297 LUMO: 0.68301 factor:1 | -1 (0.01124) | -1 | -1 |
| G: -5717.87902 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.30989 HOMO: -6.01916 LUMO: 0.56328 factor:1 | 1 (-0.06517) | -1 | -1 |
| G: -5717.87902 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.25359 HOMO: -6.05181 LUMO: 0.35103 factor:1 | 1 (-0.00887) | -1 | -1 |
| G: -5717.87902 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.04606 HOMO: -6.08447 LUMO: 0.48436 factor:1 | -1 (2.19865) | -1 | -1 |
| G: -5717.87902 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11979.83213 HOMO: -5.86950 LUMO: 0.36735 factor:1 | -1 (2.41259) | -1 | -1 |
| G: -5717.87902 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.29966 HOMO: -5.33615 LUMO: 0.65852 factor:1 | -1 (0.94505) | -1 | -1 |
| G: -5717.87902 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.95464 HOMO: -5.36064 LUMO: 0.86804 factor:1 | -1 (0.29007) | -1 | -1 |
| G: -5717.87902 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.04796 HOMO: -5.74160 LUMO: 0.64491 factor:1 | -1 (1.19676) | -1 | -1 |
| G: -5717.87902 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.73859 HOMO: -5.23003 LUMO: 0.66124 factor:1 | -1 (1.50612) | -1 | -1 |
| G: -5717.87902 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.48553 HOMO: -5.77698 LUMO: 0.84083 factor:1 | -1 (1.75919) | -1 | -1 |
| G: -5717.87902 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.37834 HOMO: -5.60555 LUMO: 0.84355 factor:1 | -1 (1.86637) | -1 | -1 |
| G: -5717.87902 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.16827 HOMO: -7.11578 LUMO: -1.62452 factor:1 | -1 (2.07645) | -1 | -1 |
| G: -5717.87902 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.08424 HOMO: -7.23279 LUMO: -1.63813 factor:1 | -1 (2.16048) | -1 | -1 |
| G: -5717.87902 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.35264 HOMO: -6.68312 LUMO: -0.88709 factor:1 | -1 (0.89207) | -1 | -1 |
| G: -5717.87902 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.18825 HOMO: -6.99333 LUMO: -0.88709 factor:1 | -1 (0.05646) | -1 | -1 |
| G: -5717.87902 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.02574 HOMO: -7.40694 LUMO: 0.11973 factor:1 | -1 (0.21897) | 1 | 1 |
| G: -5717.87902 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.14342 HOMO: -6.74026 LUMO: -0.72927 factor:1 | -1 (1.10130) | -1 | -1 |
| G: -5717.87902 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.08096 HOMO: -6.67223 LUMO: -0.70750 factor:1 | -1 (0.16376) | -1 | -1 |
| G: -5717.87902 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.20192 HOMO: -7.06952 LUMO: -1.40139 factor:1 | -1 (1.04279) | -1 | -1 |
| G: -5717.87902 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.11888 HOMO: -7.21374 LUMO: -1.13199 factor:1 | -1 (2.12584) | -1 | -1 |
| G: -5717.87902 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.16253 HOMO: -6.54706 LUMO: -1.34424 factor:1 | -1 (2.08219) | -1 | -1 |
| G: -5717.87902 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.73946 HOMO: -7.51851 LUMO: -1.05852 factor:1 | -1 (1.50525) | -1 | -1 |
| G: -5717.87902 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.63413 HOMO: -7.07224 LUMO: -1.89391 factor:1 | -1 (1.61059) | -1 | -1 |
| G: -5717.87902 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11979.95567 HOMO: -6.65863 LUMO: -0.46804 factor:1 | -1 (2.28905) | -1 | -1 |
| G: -5717.87902 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.19428 HOMO: -7.24367 LUMO: 0.29388 factor:1 | -1 (2.05043) | 1 | 1 |
| G: -5717.87902 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11979.49718 HOMO: -7.02326 LUMO: -0.87893 factor:1 | -1 (2.74753) | -1 | -1 |
| G: -5717.87902 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11979.18738 HOMO: -6.88176 LUMO: 0.71566 factor:1 | -1 (3.05734) | -1 | -1 |
| G: -5717.87902 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.06731 HOMO: -6.46543 LUMO: 1.01498 factor:1 | -1 (2.17740) | -1 | -1 |
| G: -5717.87902 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.65767 HOMO: -6.30760 LUMO: 0.17687 factor:1 | -1 (1.58705) | -1 | -1 |
| G: -5717.87902 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.62218 HOMO: -6.73210 LUMO: -1.06941 factor:1 | -1 (1.62253) | -1 | -1 |
| G: -5717.87902 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.87040 HOMO: -6.83550 LUMO: -0.75920 factor:1 | -1 (1.37431) | -1 | -1 |
| G: -5717.87902 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.74635 HOMO: -6.94707 LUMO: 0.42178 factor:1 | -1 (1.49837) | -1 | -1 |
| G: -5717.87902 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.40139 HOMO: -6.77019 LUMO: -0.38096 factor:1 | -1 (1.84333) | -1 | -1 |
| G: -5717.87902 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.61100 HOMO: -7.34163 LUMO: 0.35103 factor:1 | -1 (1.63372) | 1 | 1 |
| G: -5717.87902 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11979.99422 HOMO: -6.87632 LUMO: -0.87349 factor:1 | -1 (2.25049) | -1 | -1 |
| G: -5717.87902 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.96243 HOMO: -7.06952 LUMO: -1.47214 factor:1 | -1 (1.28228) | -1 | -1 |
| G: -5717.87902 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.85658 HOMO: -6.58788 LUMO: -0.37824 factor:1 | -1 (1.38813) | -1 | -1 |
| G: -5717.87902 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.67560 HOMO: -6.92802 LUMO: -1.24900 factor:1 | -1 (1.56912) | -1 | -1 |
| G: -5717.87902 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.61647 HOMO: -7.01237 LUMO: -1.31975 factor:1 | -1 (1.62825) | -1 | -1 |
| G: -5717.87902 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.00529 HOMO: -6.74842 LUMO: 0.45987 factor:1 | -1 (1.23942) | -1 | -1 |
| G: -5717.87902 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.14478 HOMO: -6.53890 LUMO: 0.94424 factor:1 | -1 (1.09994) | -1 | -1 |
| G: -5717.87902 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.34486 HOMO: -6.52257 LUMO: -0.66940 factor:1 | -1 (0.89985) | -1 | -1 |
| G: -5717.87902 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.12491 HOMO: -6.56883 LUMO: -1.48302 factor:1 | -1 (1.11980) | -1 | -1 |
| G: -5717.87902 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.92959 HOMO: -7.21646 LUMO: 0.13061 factor:1 | -1 (1.31513) | 1 | 1 |
| G: -5717.87902 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.52689 HOMO: -6.62597 LUMO: -0.64763 factor:1 | -1 (1.71783) | -1 | -1 |
| G: -5717.87902 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.45353 HOMO: -7.38789 LUMO: 0.31021 factor:1 | -1 (1.79119) | 1 | 1 |
| G: -5717.87902 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.41206 HOMO: -6.74570 LUMO: -0.70750 factor:1 | -1 (1.83266) | -1 | -1 |
| G: -5717.87902 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.32226 HOMO: -6.95251 LUMO: -1.25989 factor:1 | -1 (1.92246) | -1 | -1 |
| G: -5717.87902 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.10074 HOMO: -7.13483 LUMO: -0.76736 factor:1 | -1 (0.14398) | -1 | -1 |
| G: -5717.87902 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.64742 HOMO: -6.93618 LUMO: -1.24628 factor:1 | 1 (-0.40270) | -1 | -1 |
| G: -5717.87902 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11983.34318 HOMO: -7.03686 LUMO: 0.26395 factor:1 | 1 (-1.09847) | -1 | -1 |
| G: -5717.87902 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.76614 HOMO: -6.52257 LUMO: -0.84355 factor:1 | 1 (-0.52142) | -1 | -1 |
| G: -5717.87902 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.11750 HOMO: -6.83278 LUMO: -0.49525 factor:1 | -1 (0.12721) | -1 | -1 |
| G: -5717.87902 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.01951 HOMO: -7.18381 LUMO: -1.64629 factor:1 | -1 (0.22520) | -1 | -1 |
| G: -5717.87902 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11983.08723 HOMO: -6.74842 LUMO: -0.81090 factor:1 | 1 (-0.84252) | -1 | -1 |
| G: -5717.87902 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11983.07733 HOMO: -7.09401 LUMO: -0.92519 factor:1 | 1 (-0.83261) | -1 | -1 |
| G: -5717.87902 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11983.09491 HOMO: -7.20285 LUMO: -0.81634 factor:1 | 1 (-0.85019) | -1 | -1 |
| G: -5717.87902 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.38651 HOMO: -6.72665 LUMO: 0.77008 factor:1 | 1 (-0.14180) | -1 | -1 |
| G: -5717.87902 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.45819 HOMO: -6.80829 LUMO: 0.86532 factor:1 | 1 (-0.21347) | -1 | -1 |
| G: -5717.87902 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11983.05534 HOMO: -6.20964 LUMO: 0.99866 factor:1 | 1 (-0.81063) | -1 | -1 |
| G: -5717.87902 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11983.47415 HOMO: -6.52801 LUMO: 1.07757 factor:1 | 1 (-1.22944) | -1 | -1 |
| G: -5717.87902 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11983.19978 HOMO: -6.74298 LUMO: -0.67756 factor:1 | 1 (-0.95507) | -1 | -1 |
| G: -5717.87902 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.57245 HOMO: -7.43959 LUMO: 0.03265 factor:1 | 1 (-0.32773) | 1 | 1 |
| G: -5717.87902 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11983.21910 HOMO: -6.46815 LUMO: -0.29933 factor:1 | 1 (-0.97439) | -1 | -1 |
| G: -5717.87902 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11983.65837 HOMO: -6.70489 LUMO: -0.97145 factor:1 | 1 (-1.41366) | -1 | -1 |
| G: -5717.87902 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.55163 HOMO: -6.30216 LUMO: -1.39322 factor:1 | 1 (-0.30692) | -1 | -1 |
| G: -5717.87902 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.85039 HOMO: -7.01782 LUMO: -1.07485 factor:1 | 1 (-0.60567) | -1 | -1 |
| G: -5717.87902 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11983.62621 HOMO: -6.93074 LUMO: 0.25851 factor:1 | 1 (-1.38149) | -1 | -1 |
| G: -5717.87902 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.52436 HOMO: -7.07224 LUMO: 0.09524 factor:1 | -1 (1.72036) | 1 | 1 |
| G: -5717.87902 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.25452 HOMO: -6.62325 LUMO: -0.45443 factor:1 | -1 (0.99020) | -1 | -1 |
| G: -5717.87902 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.28350 HOMO: -7.09945 LUMO: -1.20274 factor:1 | -1 (0.96121) | -1 | -1 |
| G: -5717.87902 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11983.21687 HOMO: -6.56067 LUMO: -1.39322 factor:1 | 1 (-0.97215) | -1 | -1 |
| G: -5717.87902 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.65114 HOMO: -6.75387 LUMO: -0.72654 factor:1 | 1 (-0.40643) | -1 | -1 |
| G: -5717.87902 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11983.24718 HOMO: -6.28583 LUMO: -2.35651 factor:1 | 1 (-1.00247) | -1 | -1 |
| G: -5717.87902 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.82168 HOMO: -6.55522 LUMO: -1.33608 factor:1 | 1 (-0.57696) | -1 | -1 |
| G: -5717.87902 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11983.59957 HOMO: -7.19741 LUMO: -0.93607 factor:1 | 1 (-1.35485) | -1 | -1 |
| G: -5717.87902 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11983.15075 HOMO: -6.39740 LUMO: -1.14832 factor:1 | 1 (-0.90603) | -1 | -1 |
| G: -5717.87902 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.32414 HOMO: -7.11850 LUMO: -0.97417 factor:1 | -1 (1.92058) | -1 | -1 |
| G: -5717.87902 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.41313 HOMO: -6.57699 LUMO: -1.14016 factor:1 | 1 (-0.16841) | -1 | -1 |
| G: -5717.87902 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.56369 HOMO: -6.57699 LUMO: -1.31975 factor:1 | 1 (-0.31897) | -1 | -1 |
| G: -5717.87902 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.71817 HOMO: -6.69128 LUMO: -0.76736 factor:1 | 1 (-0.47345) | -1 | -1 |
| G: -5717.87902 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.56861 HOMO: -7.25728 LUMO: 0.29660 factor:1 | 1 (-0.32390) | 1 | 1 |
| G: -5717.87902 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.66709 HOMO: -6.37019 LUMO: -0.95240 factor:1 | 1 (-0.42238) | -1 | -1 |
| G: -5717.87902 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.96698 HOMO: -6.48447 LUMO: -0.55511 factor:1 | -1 (1.27774) | -1 | -1 |
| G: -5717.87902 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.47510 HOMO: -6.37291 LUMO: -0.78641 factor:1 | -1 (0.76962) | -1 | -1 |
| G: -5717.87902 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.11151 HOMO: -6.65863 LUMO: -0.69933 factor:1 | -1 (2.13321) | -1 | -1 |
| G: -5717.87902 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.43480 HOMO: -6.44638 LUMO: -0.16055 factor:1 | -1 (1.80991) | -1 | -1 |
| G: -5717.87902 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.29515 HOMO: -6.41917 LUMO: -0.20136 factor:1 | -1 (0.94957) | -1 | -1 |
| G: -5717.87902 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.38244 HOMO: -7.33347 LUMO: 0.12789 factor:1 | -1 (0.86227) | 1 | 1 |
| G: -5717.87902 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.09753 HOMO: -6.70489 LUMO: -0.52518 factor:1 | -1 (0.14719) | -1 | -1 |
| G: -5717.87902 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.31681 HOMO: -7.25183 LUMO: 0.32109 factor:1 | -1 (0.92791) | 1 | 1 |
| G: -5717.87902 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.67216 HOMO: -7.29265 LUMO: 0.28028 factor:1 | -1 (0.57255) | 1 | 1 |
| G: -5717.87902 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.19991 HOMO: -6.57155 LUMO: -0.51702 factor:1 | -1 (1.04481) | -1 | -1 |
| G: -5717.87902 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11983.05121 HOMO: -7.08040 LUMO: 0.39729 factor:1 | 1 (-0.80649) | 1 | 1 |
| G: -5717.87902 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11983.14049 HOMO: -6.24501 LUMO: -0.44627 factor:1 | 1 (-0.89577) | -1 | -1 |
| G: -5717.87902 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11983.09551 HOMO: -6.73754 LUMO: -0.45443 factor:1 | 1 (-0.85079) | -1 | -1 |
| G: -5717.87902 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.05489 HOMO: -6.24501 LUMO: 0.38096 factor:1 | -1 (0.18983) | -1 | -1 |
| G: -5717.87902 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.27715 HOMO: -6.86815 LUMO: -0.91974 factor:1 | 1 (-0.03244) | -1 | -1 |
| G: -5717.87902 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.78053 HOMO: -7.40150 LUMO: 0.36191 factor:1 | 1 (-0.53582) | 1 | 1 |
| G: -5717.87902 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.78862 HOMO: -6.44094 LUMO: -0.64219 factor:1 | -1 (0.45609) | -1 | -1 |
| G: -5717.87902 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.15248 HOMO: -6.69944 LUMO: -0.80001 factor:1 | -1 (1.09224) | -1 | -1 |
| G: -5717.87902 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.11608 HOMO: -6.61509 LUMO: -0.70750 factor:1 | -1 (2.12864) | -1 | -1 |
| G: -5717.87902 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.49955 HOMO: -7.52123 LUMO: 0.06803 factor:1 | 1 (-0.25483) | 1 | 1 |
| G: -5717.87902 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.58156 HOMO: -7.34163 LUMO: 0.30477 factor:1 | 1 (-0.33685) | 1 | 1 |
| G: -5717.87902 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.27476 HOMO: -6.68584 LUMO: -0.78641 factor:1 | 1 (-0.03004) | -1 | -1 |
| G: -5717.87902 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.37228 HOMO: -6.53890 LUMO: -0.50885 factor:1 | 1 (-0.12757) | -1 | -1 |
| G: -5717.87902 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.45160 HOMO: -6.75659 LUMO: -0.68845 factor:1 | 1 (-0.20689) | -1 | -1 |
| G: -5717.87902 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.43439 HOMO: -7.08857 LUMO: 0.43266 factor:1 | -1 (0.81033) | 1 | 1 |
| G: -5717.87902 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.11205 HOMO: -6.28583 LUMO: -0.46804 factor:1 | -1 (2.13267) | -1 | -1 |
| G: -5717.87902 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.24043 HOMO: -6.50080 LUMO: -0.24762 factor:1 | -1 (2.00428) | -1 | -1 |
| G: -5717.87902 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.24035 HOMO: -6.45454 LUMO: -0.58504 factor:1 | -1 (2.00436) | -1 | -1 |
| G: -5717.87902 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.16792 HOMO: -7.20558 LUMO: 0.20953 factor:1 | -1 (0.07679) | 1 | 1 |
| G: -5717.87902 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.36726 HOMO: -6.35930 LUMO: -0.20681 factor:1 | -1 (0.87746) | -1 | -1 |
| G: -5717.87902 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.21960 HOMO: -6.36202 LUMO: -0.14422 factor:1 | -1 (0.02512) | -1 | -1 |
| G: -5717.87902 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.42573 HOMO: -6.20692 LUMO: 1.97827 factor:1 | -1 (0.81898) | -1 | -1 |
| G: -5717.87902 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.10475 HOMO: -6.48719 LUMO: 1.74153 factor:1 | -1 (1.13997) | -1 | -1 |
| G: -5717.87902 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.36859 HOMO: -6.84638 LUMO: 1.88575 factor:1 | -1 (0.87612) | -1 | -1 |
| G: -5717.87902 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.19430 HOMO: -5.90759 LUMO: 2.00820 factor:1 | -1 (1.05041) | -1 | -1 |
| G: -5717.87902 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.65698 HOMO: -6.56339 LUMO: 1.99732 factor:1 | -1 (1.58773) | -1 | -1 |
| G: -5717.87902 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.59329 HOMO: -6.20692 LUMO: 1.75241 factor:1 | 1 (-0.34858) | -1 | -1 |
| G: -5717.87902 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.60576 HOMO: -6.16882 LUMO: 1.94017 factor:1 | 1 (-0.36104) | -1 | -1 |
| G: -5717.87902 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11983.55979 HOMO: -6.80829 LUMO: 1.78507 factor:1 | 1 (-1.31507) | -1 | -1 |
| G: -5717.87902 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.41783 HOMO: -6.58243 LUMO: 1.78235 factor:1 | 1 (-0.17312) | -1 | -1 |
| G: -5717.87902 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11983.16645 HOMO: -5.85045 LUMO: 1.82316 factor:1 | 1 (-0.92173) | -1 | -1 |
| G: -5717.87902 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.64192 HOMO: -5.93752 LUMO: 1.56465 factor:1 | 1 (-0.39720) | -1 | -1 |
| G: -5717.87902 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.05013 HOMO: -6.59604 LUMO: -0.53334 factor:1 | -1 (0.19459) | -1 | -1 |
| G: -5717.87902 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11979.98783 HOMO: -7.06135 LUMO: 0.29660 factor:1 | -1 (2.25689) | 1 | 1 |
| G: -5717.87902 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.98276 HOMO: -6.50352 LUMO: 1.61908 factor:1 | -1 (1.26196) | -1 | -1 |
| G: -5717.87902 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.48344 HOMO: -6.68040 LUMO: -0.60681 factor:1 | 1 (-0.23873) | -1 | -1 |
| G: -5717.87902 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.57150 HOMO: -6.93618 LUMO: -1.09662 factor:1 | 1 (-0.32678) | -1 | -1 |
| G: -5717.87902 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.30175 HOMO: -6.72121 LUMO: -1.14016 factor:1 | 1 (-0.05704) | -1 | -1 |
| G: -5717.87902 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.45337 HOMO: -7.12394 LUMO: -1.24900 factor:1 | 1 (-0.20866) | -1 | -1 |
| G: -5717.87902 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.49101 HOMO: -6.71305 LUMO: -0.71566 factor:1 | 1 (-0.24629) | -1 | -1 |
| G: -5717.87902 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.27369 HOMO: -7.09401 LUMO: -0.86532 factor:1 | 1 (-0.02898) | -1 | -1 |
| G: -5717.87902 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.46358 HOMO: -7.08584 LUMO: -0.92519 factor:1 | 1 (-0.21886) | -1 | -1 |
| G: -5717.87902 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.72993 HOMO: -7.05591 LUMO: 0.11973 factor:1 | -1 (0.51479) | -1 | -1 |
| G: -5717.87902 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.56937 HOMO: -7.14843 LUMO: -1.58370 factor:1 | 1 (-0.32466) | -1 | -1 |
| G: -5717.87902 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.41957 HOMO: -7.36884 LUMO: -1.97010 factor:1 | -1 (1.82515) | -1 | -1 |
| G: -5717.87902 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.19559 HOMO: -6.81373 LUMO: -1.72248 factor:1 | -1 (2.04913) | -1 | -1 |
| G: -5717.87902 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.36144 HOMO: -6.87360 LUMO: -1.03947 factor:1 | -1 (1.88327) | -1 | -1 |
| G: -5717.87902 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.14567 HOMO: -7.02870 LUMO: -0.87349 factor:1 | -1 (0.09905) | -1 | -1 |
| G: -5717.87902 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.47183 HOMO: -7.16476 LUMO: -1.18097 factor:1 | -1 (0.77288) | -1 | -1 |
| G: -5717.87902 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.32119 HOMO: -7.51851 LUMO: 0.07891 factor:1 | -1 (0.92353) | 1 | 1 |
| G: -5717.87902 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.43609 HOMO: -7.04231 LUMO: -0.83539 factor:1 | 1 (-0.19138) | -1 | -1 |
| G: -5717.87902 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.89977 HOMO: -6.83278 LUMO: -0.60137 factor:1 | 1 (-0.65506) | -1 | -1 |
| G: -5717.87902 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.52913 HOMO: -6.89809 LUMO: -1.19186 factor:1 | 1 (-0.28441) | -1 | -1 |
| G: -5717.87902 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.44891 HOMO: -7.16476 LUMO: -0.79185 factor:1 | 1 (-0.20419) | -1 | -1 |
| G: -5717.87902 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.17527 HOMO: -6.97156 LUMO: -1.25444 factor:1 | -1 (0.06944) | -1 | -1 |
| G: -5717.87902 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.07513 HOMO: -6.84366 LUMO: -0.88437 factor:1 | -1 (0.16958) | -1 | -1 |
| G: -5717.87902 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.70883 HOMO: -6.91986 LUMO: -1.12655 factor:1 | 1 (-0.46412) | -1 | -1 |
| G: -5717.87902 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.46227 HOMO: -6.49536 LUMO: -0.29660 factor:1 | 1 (-0.21756) | -1 | -1 |
| G: -5717.87902 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.31193 HOMO: -6.74842 LUMO: 0.42450 factor:1 | 1 (-0.06721) | -1 | -1 |
| G: -5717.87902 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.72627 HOMO: -7.34435 LUMO: 0.32109 factor:1 | 1 (-0.48156) | 1 | 1 |
| G: -5717.87902 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.00021 HOMO: -7.16476 LUMO: 0.28572 factor:1 | -1 (2.24450) | 1 | 1 |
| G: -5717.87902 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.76315 HOMO: -6.74298 LUMO: -0.43538 factor:1 | -1 (0.48156) | -1 | -1 |
| G: -5717.87902 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.12237 HOMO: -7.19469 LUMO: -1.61091 factor:1 | -1 (0.12234) | -1 | -1 |
| G: -5717.87902 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.29158 HOMO: -7.35252 LUMO: -1.78235 factor:1 | -1 (0.95313) | -1 | -1 |
| G: -5717.87902 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.05408 HOMO: -7.25456 LUMO: -1.66806 factor:1 | -1 (1.19063) | -1 | -1 |
| G: -5717.87902 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.20297 HOMO: -7.54844 LUMO: -1.07213 factor:1 | -1 (0.04174) | -1 | -1 |
| G: -5717.87902 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.33972 HOMO: -7.21918 LUMO: -1.55377 factor:1 | -1 (0.90500) | -1 | -1 |
| G: -5717.87902 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.21609 HOMO: -7.01782 LUMO: -1.60547 factor:1 | -1 (0.02863) | -1 | -1 |
| G: -5717.87902 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.26864 HOMO: -7.21646 LUMO: -1.53472 factor:1 | -1 (0.97607) | -1 | -1 |
| G: -5717.87902 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.79576 HOMO: -6.73754 LUMO: -1.37417 factor:1 | -1 (1.44895) | -1 | -1 |
| G: -5717.87902 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.08738 HOMO: -6.78924 LUMO: 0.66396 factor:1 | -1 (0.15734) | -1 | -1 |
| G: -5717.87902 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.21234 HOMO: -6.82734 LUMO: 0.61226 factor:1 | -1 (1.03237) | -1 | -1 |
| G: -5717.87902 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.01362 HOMO: -6.74026 LUMO: 0.65579 factor:1 | -1 (1.23110) | -1 | -1 |
| G: -5717.87902 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.35159 HOMO: -7.10489 LUMO: -1.30887 factor:1 | -1 (1.89312) | -1 | -1 |
| G: -5717.87902 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.41304 HOMO: -7.05047 LUMO: 0.42722 factor:1 | 1 (-0.16833) | -1 | -1 |
| G: -5717.87902 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.36385 HOMO: -6.61237 LUMO: 1.30887 factor:1 | 1 (-0.11913) | -1 | -1 |
| G: -5717.87902 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.17231 HOMO: -7.05863 LUMO: 0.59049 factor:1 | -1 (0.07241) | -1 | -1 |
| G: -5717.87902 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.82854 HOMO: -6.26406 LUMO: 0.78641 factor:1 | 1 (-0.58382) | -1 | -1 |
| G: -5717.87902 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.48211 HOMO: -6.70489 LUMO: 0.67756 factor:1 | 1 (-0.23739) | -1 | -1 |
| G: -5717.87902 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.54567 HOMO: -6.78652 LUMO: -0.94968 factor:1 | 1 (-0.30096) | -1 | -1 |
| G: -5717.87902 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.45035 HOMO: -6.36202 LUMO: -0.94424 factor:1 | 1 (-0.20564) | -1 | -1 |
| G: -5717.87902 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.60684 HOMO: -6.81645 LUMO: -1.09934 factor:1 | 1 (-0.36213) | -1 | -1 |
| G: -5717.87902 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.17806 HOMO: -7.07224 LUMO: 0.85988 factor:1 | -1 (2.06665) | 1 | 1 |
| G: -5717.87902 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.06337 HOMO: -7.02326 LUMO: 1.10206 factor:1 | -1 (2.18135) | -1 | -1 |
| G: -5717.87902 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.00359 HOMO: -6.71305 LUMO: 0.84627 factor:1 | -1 (0.24112) | -1 | -1 |
| G: -5717.87902 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.11699 HOMO: -7.27360 LUMO: 0.88165 factor:1 | -1 (1.12772) | 1 | 1 |
| G: -5717.87902 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.17620 HOMO: -6.84911 LUMO: 0.59865 factor:1 | -1 (0.06852) | -1 | -1 |
| G: -5717.87902 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.48124 HOMO: -6.75114 LUMO: -2.49801 factor:1 | -1 (0.76347) | -1 | -1 |
| G: -5717.87902 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.81039 HOMO: -6.97156 LUMO: 0.53606 factor:1 | -1 (0.43432) | -1 | -1 |
| G: -5717.87902 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.25233 HOMO: -6.54434 LUMO: 0.73199 factor:1 | 1 (-0.00762) | -1 | -1 |
| G: -5717.87902 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.33716 HOMO: -6.21236 LUMO: 0.99866 factor:1 | -1 (0.90755) | -1 | -1 |
| G: -5717.87902 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.54614 HOMO: -6.34025 LUMO: 0.50341 factor:1 | -1 (0.69857) | -1 | -1 |
| G: -5717.87902 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.54640 HOMO: -6.59876 LUMO: -0.69389 factor:1 | -1 (1.69832) | -1 | -1 |
| G: -5717.87902 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.06527 HOMO: -6.54978 LUMO: -1.00682 factor:1 | -1 (2.17944) | -1 | -1 |
| G: -5717.87902 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.24786 HOMO: -6.82462 LUMO: -0.98777 factor:1 | -1 (1.99685) | -1 | -1 |
| G: -5717.87902 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.59723 HOMO: -6.85455 LUMO: -0.68573 factor:1 | -1 (1.64749) | -1 | -1 |
| G: -5717.87902 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.40740 HOMO: -7.55388 LUMO: -0.03265 factor:1 | -1 (1.83731) | 1 | 1 |
| G: -5717.87902 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.96932 HOMO: -6.77019 LUMO: -0.71838 factor:1 | -1 (1.27540) | -1 | -1 |
| G: -5717.87902 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.74863 HOMO: -6.84911 LUMO: -1.25444 factor:1 | -1 (1.49608) | -1 | -1 |
| G: -5717.87902 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.92581 HOMO: -6.95251 LUMO: -1.03675 factor:1 | -1 (1.31891) | -1 | -1 |
| G: -5717.87902 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.60169 HOMO: -6.80829 LUMO: -0.77280 factor:1 | -1 (1.64302) | -1 | -1 |
| G: -5717.87902 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.16401 HOMO: -6.94162 LUMO: -0.94151 factor:1 | -1 (1.08070) | -1 | -1 |
| G: -5717.87902 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.76912 HOMO: -6.89809 LUMO: -0.90886 factor:1 | -1 (1.47559) | -1 | -1 |
| G: -5717.87902 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.40155 HOMO: -6.85183 LUMO: -0.88981 factor:1 | -1 (1.84316) | -1 | -1 |
| G: -5717.87902 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11979.86826 HOMO: -6.51985 LUMO: -0.84627 factor:1 | -1 (2.37645) | -1 | -1 |
| G: -5717.87902 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.35842 HOMO: -6.83278 LUMO: -1.08029 factor:1 | -1 (1.88629) | -1 | -1 |
| G: -5717.87902 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11979.85248 HOMO: -6.91986 LUMO: 0.66396 factor:1 | -1 (2.39223) | -1 | -1 |
| G: -5717.87902 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.00446 HOMO: -6.94162 LUMO: 0.50885 factor:1 | -1 (2.24026) | -1 | -1 |
| G: -5717.87902 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.21317 HOMO: -6.94435 LUMO: 0.80546 factor:1 | -1 (2.03155) | -1 | -1 |
| G: -5717.87902 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11979.80954 HOMO: -6.74298 LUMO: -0.81634 factor:1 | -1 (2.43517) | -1 | -1 |
| G: -5717.87902 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11979.92533 HOMO: -7.04503 LUMO: 1.15921 factor:1 | -1 (2.31939) | -1 | -1 |
| G: -5717.87902 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.23722 HOMO: -6.76475 LUMO: 0.75920 factor:1 | -1 (2.00749) | -1 | -1 |
| G: -5717.87902 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11979.89803 HOMO: -7.05047 LUMO: 0.68845 factor:1 | -1 (2.34668) | -1 | -1 |
| G: -5717.87902 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.82959 HOMO: -7.12666 LUMO: 0.60681 factor:1 | -1 (1.41513) | 1 | 1 |
| G: -5717.87902 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.96543 HOMO: -6.90897 LUMO: -1.22723 factor:1 | -1 (1.27929) | -1 | -1 |
| G: -5717.87902 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.52041 HOMO: -7.10761 LUMO: 0.58232 factor:1 | -1 (1.72430) | 1 | 1 |
| G: -5717.87902 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.59268 HOMO: -6.57427 LUMO: 0.71294 factor:1 | -1 (1.65203) | -1 | -1 |
| G: -5717.87902 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.20765 HOMO: -6.22597 LUMO: 0.99322 factor:1 | -1 (0.03706) | -1 | -1 |
| G: -5717.87902 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.73686 HOMO: -6.83550 LUMO: -0.77825 factor:1 | 1 (-0.49215) | -1 | -1 |
| G: -5717.87902 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.16912 HOMO: -7.14843 LUMO: 0.44627 factor:1 | -1 (0.07559) | 1 | 1 |
| G: -5717.87902 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.12441 HOMO: -7.08040 LUMO: 0.78913 factor:1 | -1 (0.12030) | 1 | 1 |
| G: -5717.87902 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.34866 HOMO: -6.81373 LUMO: -0.93879 factor:1 | 1 (-0.10395) | -1 | -1 |
| G: -5717.87902 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.18346 HOMO: -6.95251 LUMO: 0.22585 factor:1 | -1 (0.06125) | -1 | -1 |
| G: -5717.87902 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.43057 HOMO: -7.13483 LUMO: -1.25444 factor:1 | 1 (-0.18585) | -1 | -1 |
| G: -5717.87902 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.35489 HOMO: -6.37835 LUMO: -1.54289 factor:1 | 1 (-0.11018) | -1 | -1 |
| G: -5717.87902 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.83690 HOMO: -6.53617 LUMO: -1.43948 factor:1 | -1 (0.40782) | -1 | -1 |
| G: -5717.87902 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.24251 HOMO: -6.38379 LUMO: 0.16055 factor:1 | -1 (0.00220) | -1 | -1 |
| G: -5717.87902 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.20281 HOMO: -6.53617 LUMO: 0.15783 factor:1 | -1 (0.04191) | -1 | -1 |
| G: -5717.87902 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11979.82674 HOMO: -6.79740 LUMO: -0.17960 factor:1 | -1 (2.41798) | -1 | -1 |
| G: -5717.87902 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.46358 HOMO: -6.26678 LUMO: -0.41361 factor:1 | -1 (0.78113) | -1 | -1 |
| G: -5717.87902 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.88357 HOMO: -6.35658 LUMO: -0.24218 factor:1 | -1 (1.36114) | -1 | -1 |
| G: -5717.87902 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.05372 HOMO: -6.48175 LUMO: -0.71566 factor:1 | -1 (0.19100) | -1 | -1 |
| G: -5717.87902 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.17920 HOMO: -6.21508 LUMO: -0.40001 factor:1 | -1 (1.06552) | -1 | -1 |
| G: -5717.87902 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.32892 HOMO: -6.51985 LUMO: -0.32654 factor:1 | -1 (0.91580) | -1 | -1 |
| G: -5717.87902 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.55826 HOMO: -6.45182 LUMO: -0.66396 factor:1 | -1 (1.68645) | -1 | -1 |
| G: -5717.87902 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.89508 HOMO: -6.51441 LUMO: -0.65307 factor:1 | -1 (0.34964) | -1 | -1 |
| G: -5717.87902 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.04491 HOMO: -6.57971 LUMO: -0.92519 factor:1 | -1 (1.19980) | -1 | -1 |
| G: -5717.87902 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.28541 HOMO: -6.67223 LUMO: -0.58232 factor:1 | -1 (1.95930) | -1 | -1 |
| G: -5717.87902 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.00726 HOMO: -6.10351 LUMO: -0.45987 factor:1 | -1 (2.23746) | -1 | -1 |
| G: -5717.87902 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.41739 HOMO: -6.13889 LUMO: -0.50341 factor:1 | -1 (1.82733) | -1 | -1 |
| G: -5717.87902 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.25504 HOMO: -6.63141 LUMO: -0.28300 factor:1 | -1 (0.98968) | -1 | -1 |
| G: -5717.87902 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.86774 HOMO: -6.37563 LUMO: -0.22858 factor:1 | -1 (1.37698) | -1 | -1 |
| G: -5717.87902 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.81707 HOMO: -6.37019 LUMO: 0.11429 factor:1 | -1 (1.42765) | -1 | -1 |
| G: -5717.87902 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.57445 HOMO: -6.23957 LUMO: 0.28844 factor:1 | -1 (1.67026) | -1 | -1 |
| G: -5717.87902 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.09841 HOMO: -6.41372 LUMO: -0.53879 factor:1 | -1 (1.14631) | -1 | -1 |
| G: -5717.87902 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.36411 HOMO: -7.06680 LUMO: 0.32654 factor:1 | -1 (1.88061) | 1 | 1 |
| G: -5717.87902 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.23709 HOMO: -6.50896 LUMO: -0.73743 factor:1 | -1 (2.00763) | -1 | -1 |
| G: -5717.87902 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.16187 HOMO: -6.42189 LUMO: -0.28572 factor:1 | -1 (2.08284) | -1 | -1 |
| G: -5717.87902 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.10478 HOMO: -6.79740 LUMO: -0.25851 factor:1 | -1 (2.13993) | -1 | -1 |
| G: -5717.87902 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.31872 HOMO: -6.32393 LUMO: 0.17960 factor:1 | -1 (1.92599) | -1 | -1 |
| G: -5717.87902 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.15710 HOMO: -6.65046 LUMO: 0.03537 factor:1 | -1 (1.08761) | -1 | -1 |
| G: -5717.87902 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.52421 HOMO: -6.60148 LUMO: 0.07619 factor:1 | -1 (0.72050) | -1 | -1 |
| G: -5717.87902 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.76760 HOMO: -6.57971 LUMO: 0.11429 factor:1 | -1 (1.47712) | -1 | -1 |
| G: -5717.87902 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.22483 HOMO: -6.88448 LUMO: -1.21907 factor:1 | -1 (1.01988) | -1 | -1 |
| G: -5717.87902 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.02524 HOMO: -6.97700 LUMO: 0.36463 factor:1 | -1 (1.21948) | -1 | -1 |
| G: -5717.87902 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.36288 HOMO: -6.73210 LUMO: -0.84083 factor:1 | -1 (0.88184) | -1 | -1 |
| G: -5717.87902 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.91389 HOMO: -6.21236 LUMO: -0.68845 factor:1 | -1 (1.33083) | -1 | -1 |
| G: -5717.87902 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.40829 HOMO: -6.35658 LUMO: -0.82995 factor:1 | -1 (0.83642) | -1 | -1 |
| G: -5717.87902 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.96420 HOMO: -6.75114 LUMO: -0.94424 factor:1 | -1 (1.28051) | -1 | -1 |
| G: -5717.87902 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.59042 HOMO: -6.74026 LUMO: -1.46125 factor:1 | -1 (0.65430) | -1 | -1 |
| G: -5717.87902 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.26048 HOMO: -7.06952 LUMO: 0.91974 factor:1 | -1 (0.98424) | 1 | 1 |
| G: -5717.87902 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.63605 HOMO: -7.08857 LUMO: 0.74559 factor:1 | -1 (0.60866) | 1 | 1 |
| G: -5717.87902 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.67651 HOMO: -6.74298 LUMO: 1.03131 factor:1 | -1 (0.56820) | -1 | -1 |
| G: -5717.87902 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.36805 HOMO: -6.74842 LUMO: -1.77962 factor:1 | -1 (0.87667) | -1 | -1 |
| G: -5717.87902 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.81331 HOMO: -6.82462 LUMO: -1.61908 factor:1 | -1 (1.43140) | -1 | -1 |
| G: -5717.87902 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.75644 HOMO: -7.17020 LUMO: -1.02043 factor:1 | -1 (1.48827) | -1 | -1 |
| G: -5717.87902 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.49386 HOMO: -6.26406 LUMO: -0.96328 factor:1 | 1 (-0.24915) | -1 | -1 |
| G: -5717.87902 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.26823 HOMO: -6.50896 LUMO: -0.38640 factor:1 | 1 (-0.02351) | -1 | -1 |
| G: -5717.87902 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.89508 HOMO: -7.27632 LUMO: -1.17553 factor:1 | -1 (0.34964) | -1 | -1 |
| G: -5717.87902 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.13647 HOMO: -6.54162 LUMO: -1.36873 factor:1 | -1 (0.10825) | -1 | -1 |
| G: -5717.87902 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.25125 HOMO: -6.42733 LUMO: -1.15648 factor:1 | 1 (-0.00653) | -1 | -1 |
| G: -5717.87902 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.22910 HOMO: -6.73754 LUMO: -2.58780 factor:1 | -1 (0.01562) | -1 | -1 |
| G: -5717.87902 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.36779 HOMO: -7.20285 LUMO: 0.75103 factor:1 | 1 (-0.12308) | 1 | 1 |
| G: -5717.87902 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11983.06062 HOMO: -6.98788 LUMO: 0.34831 factor:1 | 1 (-0.81591) | -1 | -1 |
| G: -5717.87902 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.22752 HOMO: -6.80013 LUMO: -1.11567 factor:1 | -1 (0.01720) | -1 | -1 |
| G: -5717.87902 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.81825 HOMO: -6.67767 LUMO: -0.82450 factor:1 | 1 (-0.57353) | -1 | -1 |
| G: -5717.87902 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11983.04797 HOMO: -6.84911 LUMO: -0.21497 factor:1 | 1 (-0.80325) | -1 | -1 |
| G: -5717.87902 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11983.17711 HOMO: -6.23141 LUMO: 0.21769 factor:1 | 1 (-0.93240) | -1 | -1 |
| G: -5717.87902 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.22319 HOMO: -6.68312 LUMO: 0.16327 factor:1 | -1 (0.02152) | -1 | -1 |
| G: -5717.87902 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.37849 HOMO: -7.04503 LUMO: -1.04220 factor:1 | 1 (-0.13377) | -1 | -1 |
| G: -5717.87902 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.74102 HOMO: -6.67495 LUMO: -0.71294 factor:1 | 1 (-0.49631) | -1 | -1 |
| G: -5717.87902 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.86464 HOMO: -6.70216 LUMO: -0.55239 factor:1 | 1 (-0.61993) | -1 | -1 |
| G: -5717.87902 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11983.20443 HOMO: -6.60420 LUMO: -0.71294 factor:1 | 1 (-0.95972) | -1 | -1 |
| G: -5717.87902 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.92873 HOMO: -7.40694 LUMO: 0.11973 factor:1 | 1 (-0.68401) | 1 | 1 |
| G: -5717.87902 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.22496 HOMO: -6.58788 LUMO: -0.29116 factor:1 | -1 (0.01976) | -1 | -1 |
| G: -5717.87902 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11983.08971 HOMO: -6.63686 LUMO: -0.32654 factor:1 | 1 (-0.84500) | -1 | -1 |
| G: -5717.87902 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.34243 HOMO: -6.85183 LUMO: -0.95512 factor:1 | 1 (-0.09772) | -1 | -1 |
| G: -5717.87902 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11983.23344 HOMO: -6.82189 LUMO: -0.88165 factor:1 | 1 (-0.98873) | -1 | -1 |
| G: -5717.87902 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.51740 HOMO: -6.97428 LUMO: -1.03947 factor:1 | 1 (-0.27269) | -1 | -1 |
| G: -5717.87902 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.34004 HOMO: -6.51441 LUMO: -0.05714 factor:1 | 1 (-0.09532) | -1 | -1 |
| G: -5717.87902 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.27138 HOMO: -6.61509 LUMO: -0.77008 factor:1 | 1 (-0.02667) | -1 | -1 |
| G: -5717.87902 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11983.08127 HOMO: -7.36340 LUMO: 0.29116 factor:1 | 1 (-0.83656) | 1 | 1 |
| G: -5717.87902 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11983.10685 HOMO: -6.64230 LUMO: -0.79185 factor:1 | 1 (-0.86214) | -1 | -1 |
| G: -5717.87902 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11983.39818 HOMO: -6.56883 LUMO: -1.03403 factor:1 | 1 (-1.15346) | -1 | -1 |
| G: -5717.87902 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.30591 HOMO: -6.69400 LUMO: -0.77825 factor:1 | 1 (-0.06120) | -1 | -1 |
| G: -5717.87902 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.35628 HOMO: -6.37019 LUMO: -0.79185 factor:1 | 1 (-0.11157) | -1 | -1 |
| G: -5717.87902 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.48502 HOMO: -6.49808 LUMO: -0.94424 factor:1 | 1 (-0.24030) | -1 | -1 |
| G: -5717.87902 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11983.33527 HOMO: -6.91713 LUMO: -0.75376 factor:1 | 1 (-1.09055) | -1 | -1 |
| G: -5717.87902 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11983.07738 HOMO: -7.13755 LUMO: 0.41361 factor:1 | 1 (-0.83267) | 1 | 1 |
| G: -5717.87902 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.93841 HOMO: -7.12122 LUMO: 0.39457 factor:1 | 1 (-0.69370) | 1 | 1 |
| G: -5717.87902 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.33299 HOMO: -6.59332 LUMO: -0.57144 factor:1 | 1 (-0.08827) | -1 | -1 |
| G: -5717.87902 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.74962 HOMO: -6.62325 LUMO: -0.66940 factor:1 | 1 (-0.50491) | -1 | -1 |
| G: -5717.87902 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.35345 HOMO: -6.90897 LUMO: -0.08708 factor:1 | 1 (-0.10874) | -1 | -1 |
| G: -5717.87902 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.16885 HOMO: -6.65591 LUMO: -0.81090 factor:1 | -1 (0.07587) | -1 | -1 |
| G: -5717.87902 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.28689 HOMO: -6.65318 LUMO: -0.94696 factor:1 | 1 (-0.04218) | -1 | -1 |
| G: -5717.87902 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.32613 HOMO: -6.96067 LUMO: -1.03675 factor:1 | 1 (-0.08142) | -1 | -1 |
| G: -5717.87902 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11983.21129 HOMO: -6.23141 LUMO: -0.66396 factor:1 | 1 (-0.96658) | -1 | -1 |
| G: -5717.87902 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.42681 HOMO: -6.52529 LUMO: -0.78369 factor:1 | 1 (-0.18210) | -1 | -1 |
| G: -5717.87902 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.90307 HOMO: -6.39468 LUMO: -0.40817 factor:1 | 1 (-0.65835) | -1 | -1 |
| G: -5717.87902 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.48227 HOMO: -6.76203 LUMO: -0.20409 factor:1 | 1 (-0.23756) | -1 | -1 |
| G: -5717.87902 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11983.18533 HOMO: -6.96611 LUMO: -0.90342 factor:1 | 1 (-0.94062) | -1 | -1 |
| G: -5717.87902 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11983.32865 HOMO: -6.54706 LUMO: -0.87893 factor:1 | 1 (-1.08394) | -1 | -1 |
| G: -5717.87902 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.75087 HOMO: -7.24367 LUMO: -0.97689 factor:1 | 1 (-0.50616) | -1 | -1 |
| G: -5717.87902 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.16977 HOMO: -6.61781 LUMO: 1.43404 factor:1 | -1 (0.07494) | -1 | -1 |
| G: -5717.87902 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.98340 HOMO: -6.17971 LUMO: 1.79867 factor:1 | 1 (-0.73868) | -1 | -1 |
| G: -5717.87902 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.35536 HOMO: -5.73344 LUMO: 2.13609 factor:1 | 1 (-0.11064) | -1 | -1 |
| G: -5717.87902 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.43032 HOMO: -6.72121 LUMO: 2.06807 factor:1 | 1 (-0.18561) | -1 | -1 |
| G: -5717.87902 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.15938 HOMO: -6.91169 LUMO: 2.02997 factor:1 | -1 (0.08533) | -1 | -1 |
| G: -5717.87902 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.96533 HOMO: -7.06408 LUMO: 1.41499 factor:1 | 1 (-0.72061) | 1 | 1 |
| G: -5717.87902 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.94126 HOMO: -6.94162 LUMO: -0.90070 factor:1 | -1 (1.30345) | -1 | -1 |
| G: -5717.87902 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.10401 HOMO: -7.09401 LUMO: 0.35103 factor:1 | -1 (1.14070) | 1 | 1 |
| G: -5717.87902 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.75798 HOMO: -6.78652 LUMO: 0.91974 factor:1 | -1 (0.48673) | -1 | -1 |
| G: -5717.87902 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.12984 HOMO: -6.32937 LUMO: -1.89119 factor:1 | -1 (1.11488) | -1 | -1 |
| G: -5717.87902 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.29681 HOMO: -7.12666 LUMO: -1.06397 factor:1 | -1 (0.94791) | -1 | -1 |
| G: -5717.87902 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.04958 HOMO: -6.38107 LUMO: -1.43132 factor:1 | -1 (0.19513) | -1 | -1 |
| G: -5717.87902 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.90445 HOMO: -7.09129 LUMO: 0.08980 factor:1 | 1 (-0.65974) | 1 | 1 |
| G: -5717.87902 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11983.00590 HOMO: -6.31304 LUMO: -0.57960 factor:1 | 1 (-0.76118) | -1 | -1 |
| G: -5717.87902 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11983.07863 HOMO: -6.94435 LUMO: -0.74287 factor:1 | 1 (-0.83392) | -1 | -1 |
| G: -5717.87902 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11983.15235 HOMO: -6.35658 LUMO: -1.53472 factor:1 | 1 (-0.90764) | -1 | -1 |
| G: -5717.87902 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11983.19339 HOMO: -6.39740 LUMO: -1.48846 factor:1 | 1 (-0.94867) | -1 | -1 |
| G: -5717.87902 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11983.04165 HOMO: -7.05319 LUMO: -0.33198 factor:1 | 1 (-0.79694) | -1 | -1 |
| G: -5717.87902 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11983.09844 HOMO: -6.68040 LUMO: -0.09252 factor:1 | 1 (-0.85373) | -1 | -1 |
| G: -5717.87902 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.86124 HOMO: -6.35930 LUMO: -0.43266 factor:1 | 1 (-0.61653) | -1 | -1 |
| G: -5717.87902 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11983.08653 HOMO: -6.59604 LUMO: -1.45853 factor:1 | 1 (-0.84181) | -1 | -1 |
| G: -5717.87902 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.86706 HOMO: -6.46270 LUMO: -1.49391 factor:1 | -1 (1.37766) | -1 | -1 |
| G: -5717.87902 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.03433 HOMO: -7.05863 LUMO: -1.04764 factor:1 | -1 (1.21039) | -1 | -1 |
| G: -5717.87902 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.01892 HOMO: -7.14027 LUMO: -0.81634 factor:1 | -1 (1.22579) | -1 | -1 |
| G: -5717.87902 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.84461 HOMO: -6.80285 LUMO: -0.74287 factor:1 | -1 (1.40011) | -1 | -1 |
| G: -5717.87902 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.73139 HOMO: -6.53890 LUMO: -1.13471 factor:1 | 1 (-0.48668) | -1 | -1 |
| G: -5717.87902 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.85701 HOMO: -6.49808 LUMO: -1.35513 factor:1 | -1 (0.38771) | -1 | -1 |
| G: -5717.87902 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.82992 HOMO: -6.75931 LUMO: -1.49663 factor:1 | 1 (-0.58521) | -1 | -1 |
| G: -5717.87902 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.74554 HOMO: -6.84638 LUMO: -0.77552 factor:1 | 1 (-0.50083) | -1 | -1 |
| G: -5717.87902 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.92841 HOMO: -6.65863 LUMO: -1.34696 factor:1 | -1 (0.31631) | -1 | -1 |
| G: -5717.87902 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.28741 HOMO: -6.25590 LUMO: -2.36467 factor:1 | 1 (-0.04269) | -1 | -1 |
| G: -5717.87902 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.15835 HOMO: -7.24911 LUMO: 0.33470 factor:1 | -1 (0.08637) | 1 | 1 |
| G: -5717.87902 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.80032 HOMO: -6.65863 LUMO: -0.75648 factor:1 | 1 (-0.55560) | -1 | -1 |
| G: -5717.87902 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.97810 HOMO: -6.31576 LUMO: -0.83267 factor:1 | -1 (0.26662) | -1 | -1 |
| G: -5717.87902 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.70740 HOMO: -6.64774 LUMO: -0.66124 factor:1 | -1 (0.53732) | -1 | -1 |
| G: -5717.87902 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.64851 HOMO: -6.75387 LUMO: -1.00138 factor:1 | -1 (0.59620) | -1 | -1 |
| G: -5717.87902 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.39903 HOMO: -6.52529 LUMO: -0.68301 factor:1 | 1 (-0.15432) | -1 | -1 |
| G: -5717.87902 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.48611 HOMO: -6.59332 LUMO: -0.68028 factor:1 | 1 (-0.24139) | -1 | -1 |
| G: -5717.87902 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.53988 HOMO: -5.98650 LUMO: 0.31565 factor:1 | 1 (-0.29516) | -1 | -1 |
| G: -5717.87902 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.59174 HOMO: -6.59876 LUMO: 0.22585 factor:1 | 1 (-0.34703) | -1 | -1 |
| G: -5717.87902 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.46943 HOMO: -6.72121 LUMO: 0.10340 factor:1 | 1 (-0.22471) | -1 | -1 |
| G: -5717.87902 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.53811 HOMO: -6.09807 LUMO: 0.20136 factor:1 | 1 (-0.29339) | -1 | -1 |
| G: -5717.87902 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.31364 HOMO: -6.31576 LUMO: 0.06259 factor:1 | 1 (-0.06893) | -1 | -1 |
| G: -5717.87902 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.33492 HOMO: -6.35658 LUMO: -0.58232 factor:1 | 1 (-0.09021) | -1 | -1 |
| G: -5717.87902 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.30810 HOMO: -6.34842 LUMO: -0.55783 factor:1 | -1 (0.93662) | -1 | -1 |
| G: -5717.87902 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.36449 HOMO: -6.47359 LUMO: -0.57144 factor:1 | -1 (1.88023) | -1 | -1 |
| G: -5717.87902 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.35543 HOMO: -6.42189 LUMO: -0.09796 factor:1 | -1 (1.88929) | -1 | -1 |
| G: -5717.87902 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.50011 HOMO: -6.35658 LUMO: -0.31293 factor:1 | -1 (1.74460) | -1 | -1 |
| G: -5717.87902 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.16912 HOMO: -7.35524 LUMO: 0.10340 factor:1 | -1 (0.07559) | 1 | 1 |
| G: -5717.87902 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.40723 HOMO: -7.10217 LUMO: 0.36463 factor:1 | -1 (0.83748) | 1 | 1 |
| G: -5717.87902 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.05638 HOMO: -6.43549 LUMO: -0.56872 factor:1 | -1 (0.18833) | -1 | -1 |
| G: -5717.87902 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.24369 HOMO: -6.50080 LUMO: -0.71294 factor:1 | -1 (1.00103) | -1 | -1 |
| G: -5717.87902 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.41464 HOMO: -6.59060 LUMO: -0.57960 factor:1 | -1 (1.83007) | -1 | -1 |
| G: -5717.87902 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.42523 HOMO: -6.78924 LUMO: -0.31565 factor:1 | -1 (1.81949) | -1 | -1 |
| G: -5717.87902 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.44662 HOMO: -6.35658 LUMO: 0.07891 factor:1 | 1 (-0.20191) | -1 | -1 |
| G: -5717.87902 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.89890 HOMO: -6.74026 LUMO: -0.87621 factor:1 | 1 (-0.65419) | -1 | -1 |
| G: -5717.87902 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.17821 HOMO: -6.54434 LUMO: 0.81906 factor:1 | -1 (0.06650) | -1 | -1 |
| G: -5717.87902 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.30257 HOMO: -6.66135 LUMO: 1.40955 factor:1 | 1 (-0.05785) | -1 | -1 |
| G: -5717.87902 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.36093 HOMO: -6.73754 LUMO: -2.54971 factor:1 | 1 (-0.11622) | -1 | -1 |
| G: -5717.87902 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.87458 HOMO: -6.65318 LUMO: 0.69389 factor:1 | 1 (-0.62986) | -1 | -1 |
| G: -5717.87902 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.31976 HOMO: -6.73482 LUMO: 0.62858 factor:1 | 1 (-0.07505) | -1 | -1 |
| G: -5717.87902 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.36191 HOMO: -6.83550 LUMO: 0.68573 factor:1 | 1 (-0.11720) | -1 | -1 |
| G: -5717.87902 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.17658 HOMO: -6.83278 LUMO: 0.45987 factor:1 | -1 (0.06814) | -1 | -1 |
| G: -5717.87902 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.37737 HOMO: -6.78380 LUMO: 0.68301 factor:1 | 1 (-0.13266) | -1 | -1 |
| G: -5717.87902 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11979.97384 HOMO: -6.90625 LUMO: 1.36601 factor:1 | -1 (2.27087) | -1 | -1 |
| G: -5717.87902 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11979.93188 HOMO: -6.82734 LUMO: 1.48302 factor:1 | -1 (2.31283) | -1 | -1 |
| G: -5717.87902 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.99932 HOMO: -6.44094 LUMO: -0.94424 factor:1 | -1 (0.24539) | -1 | -1 |
| G: -5717.87902 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.06556 HOMO: -6.91441 LUMO: 0.28844 factor:1 | -1 (1.17915) | -1 | -1 |
| G: -5717.87902 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.94700 HOMO: -6.49808 LUMO: -0.51157 factor:1 | -1 (0.29772) | -1 | -1 |
| G: -5717.87902 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.09038 HOMO: -7.09673 LUMO: -0.06259 factor:1 | -1 (1.15433) | 1 | 1 |
| G: -5717.87902 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.03457 HOMO: -6.77019 LUMO: 0.92247 factor:1 | -1 (1.21014) | -1 | -1 |
| G: -5717.87902 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.99910 HOMO: -6.75931 LUMO: 1.13744 factor:1 | -1 (0.24561) | -1 | -1 |
| G: -5717.87902 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.13588 HOMO: -6.15794 LUMO: 1.12383 factor:1 | -1 (1.10884) | -1 | -1 |
| G: -5717.87902 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.86249 HOMO: -6.59604 LUMO: 1.19458 factor:1 | -1 (1.38223) | -1 | -1 |
| G: -5717.87902 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.26328 HOMO: -7.09401 LUMO: 0.60137 factor:1 | -1 (0.98143) | 1 | 1 |
| G: -5717.87902 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.07438 HOMO: -6.34025 LUMO: 0.48164 factor:1 | -1 (1.17033) | -1 | -1 |
| G: -5717.87902 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.83506 HOMO: -6.72665 LUMO: -2.47624 factor:1 | -1 (1.40966) | -1 | -1 |
| G: -5717.87902 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.11631 HOMO: -6.48175 LUMO: 0.58232 factor:1 | -1 (1.12840) | -1 | -1 |
| G: -5717.87902 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.36671 HOMO: -6.94162 LUMO: 0.28300 factor:1 | -1 (0.87800) | -1 | -1 |
| G: -5717.87902 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.90959 HOMO: -6.65591 LUMO: 0.57144 factor:1 | -1 (1.33513) | -1 | -1 |
| G: -5717.87902 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.94575 HOMO: -6.58788 LUMO: -1.03947 factor:1 | -1 (1.29896) | -1 | -1 |
| G: -5717.87902 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.00161 HOMO: -7.18108 LUMO: 0.37824 factor:1 | -1 (0.24311) | 1 | 1 |
| G: -5717.87902 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.79333 HOMO: -6.63958 LUMO: -1.52112 factor:1 | -1 (0.45138) | -1 | -1 |
| G: -5717.87902 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.12558 HOMO: -6.12528 LUMO: -0.53606 factor:1 | -1 (0.11913) | -1 | -1 |
| G: -5717.87902 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.66492 HOMO: -6.22324 LUMO: -0.87893 factor:1 | -1 (0.57979) | -1 | -1 |
| G: -5717.87902 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.77358 HOMO: -6.62053 LUMO: -0.91974 factor:1 | -1 (0.47114) | -1 | -1 |
| G: -5717.87902 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.78076 HOMO: -6.84366 LUMO: -0.83811 factor:1 | -1 (0.46395) | -1 | -1 |
| G: -5717.87902 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11983.07317 HOMO: -7.26000 LUMO: 0.25851 factor:1 | 1 (-0.82845) | 1 | 1 |
| G: -5717.87902 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.24950 HOMO: -6.49536 LUMO: -0.63403 factor:1 | 1 (-0.00479) | -1 | -1 |
| G: -5717.87902 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.28828 HOMO: -6.45726 LUMO: -0.77825 factor:1 | 1 (-0.04357) | -1 | -1 |
| G: -5717.87902 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11983.06051 HOMO: -6.74570 LUMO: -0.75103 factor:1 | 1 (-0.81580) | -1 | -1 |
| G: -5717.87902 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.25212 HOMO: -7.20285 LUMO: 0.10612 factor:1 | 1 (-0.00740) | 1 | 1 |
| G: -5717.87902 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11983.16495 HOMO: -6.45182 LUMO: -0.56600 factor:1 | 1 (-0.92023) | -1 | -1 |
| G: -5717.87902 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.11824 HOMO: -6.83278 LUMO: -0.71838 factor:1 | -1 (0.12648) | -1 | -1 |
| G: -5717.87902 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.66848 HOMO: -7.01510 LUMO: -1.09662 factor:1 | 1 (-0.42376) | -1 | -1 |
| G: -5717.87902 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.49294 HOMO: -6.48719 LUMO: 0.16871 factor:1 | 1 (-0.24822) | -1 | -1 |
| G: -5717.87902 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.26771 HOMO: -7.30898 LUMO: 0.26667 factor:1 | 1 (-0.02299) | 1 | 1 |
| G: -5717.87902 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.27723 HOMO: -6.68856 LUMO: -0.78641 factor:1 | 1 (-0.03252) | -1 | -1 |
| G: -5717.87902 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.73683 HOMO: -6.56883 LUMO: -1.00682 factor:1 | 1 (-0.49212) | -1 | -1 |
| G: -5717.87902 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11983.12944 HOMO: -6.41100 LUMO: -0.48980 factor:1 | 1 (-0.88472) | -1 | -1 |
| G: -5717.87902 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.98645 HOMO: -6.52257 LUMO: -0.59865 factor:1 | -1 (0.25826) | -1 | -1 |
| G: -5717.87902 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.89630 HOMO: -6.63686 LUMO: -0.56055 factor:1 | -1 (0.34841) | -1 | -1 |
| G: -5717.87902 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.55977 HOMO: -6.79740 LUMO: -0.75376 factor:1 | 1 (-0.31505) | -1 | -1 |
| G: -5717.87902 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11983.13036 HOMO: -5.89127 LUMO: 0.22313 factor:1 | 1 (-0.88565) | -1 | -1 |
| G: -5717.87902 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.84081 HOMO: -6.34842 LUMO: 0.11429 factor:1 | 1 (-0.59609) | -1 | -1 |
| G: -5717.87902 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.61362 HOMO: -6.13617 LUMO: 1.94834 factor:1 | 1 (-0.36890) | -1 | -1 |
| G: -5717.87902 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.95470 HOMO: -6.50080 LUMO: 1.74153 factor:1 | -1 (0.29002) | -1 | -1 |
| G: -5717.87902 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.49471 HOMO: -6.33481 LUMO: 1.68438 factor:1 | 1 (-0.24999) | -1 | -1 |
| G: -5717.87902 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.06749 HOMO: -6.53073 LUMO: 1.95106 factor:1 | -1 (0.17723) | -1 | -1 |
| G: -5717.87902 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.75271 HOMO: -6.46270 LUMO: 1.89935 factor:1 | -1 (0.49201) | -1 | -1 |
| G: -5717.87902 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.89260 HOMO: -5.87222 LUMO: 1.91568 factor:1 | -1 (0.35212) | -1 | -1 |
| G: -5717.87902 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.07228 HOMO: -6.07630 LUMO: 1.81500 factor:1 | -1 (0.17244) | -1 | -1 |
| G: -5717.87902 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.84441 HOMO: -6.20964 LUMO: 1.81500 factor:1 | -1 (0.40031) | -1 | -1 |
| G: -5717.87902 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.92451 HOMO: -6.15522 LUMO: 1.90752 factor:1 | 1 (-0.67979) | -1 | -1 |
| G: -5717.87902 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.93458 HOMO: -6.11984 LUMO: 1.95378 factor:1 | 1 (-0.68986) | -1 | -1 |
| G: -5717.87902 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.91614 HOMO: -6.58516 LUMO: 2.04358 factor:1 | -1 (0.32858) | -1 | -1 |
| G: -5717.87902 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.03554 HOMO: -7.37156 LUMO: 0.24490 factor:1 | -1 (0.20917) | 1 | 1 |
| G: -5717.87902 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.17739 HOMO: -6.36474 LUMO: -0.90070 factor:1 | -1 (0.06732) | -1 | -1 |
| G: -5717.87902 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.37579 HOMO: -6.43549 LUMO: -0.40817 factor:1 | 1 (-0.13108) | -1 | -1 |
| G: -5717.87902 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.79512 HOMO: -7.32258 LUMO: 0.29388 factor:1 | 1 (-0.55040) | 1 | 1 |
| G: -5717.87902 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11983.04889 HOMO: -6.41372 LUMO: -0.20409 factor:1 | 1 (-0.80418) | -1 | -1 |
| G: -5717.87902 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.70402 HOMO: -7.18381 LUMO: 0.42722 factor:1 | 1 (-0.45930) | 1 | 1 |
| G: -5717.87902 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.77265 HOMO: -6.53890 LUMO: -0.54151 factor:1 | -1 (0.47206) | -1 | -1 |
| G: -5717.87902 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.64288 HOMO: -6.61509 LUMO: 0.08708 factor:1 | -1 (0.60183) | -1 | -1 |
| G: -5717.87902 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.82334 HOMO: -6.78108 LUMO: 2.03541 factor:1 | 1 (-0.57862) | -1 | -1 |
| G: -5717.87902 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11983.04282 HOMO: -6.50896 LUMO: 1.53472 factor:1 | 1 (-0.79811) | -1 | -1 |
| G: -5717.87902 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11983.01303 HOMO: -6.65591 LUMO: 1.80411 factor:1 | 1 (-0.76831) | -1 | -1 |
| G: -5717.87902 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.93980 HOMO: -6.64502 LUMO: 1.52112 factor:1 | 1 (-0.69509) | -1 | -1 |
| G: -5717.87902 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.86715 HOMO: -6.72938 LUMO: 1.48030 factor:1 | 1 (-0.62243) | -1 | -1 |
| G: -5717.87902 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11983.01706 HOMO: -6.16882 LUMO: 1.96466 factor:1 | 1 (-0.77234) | -1 | -1 |
| G: -5717.87902 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.95771 HOMO: -6.22597 LUMO: 1.43132 factor:1 | 1 (-0.71299) | -1 | -1 |
| G: -5717.87902 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.81920 HOMO: -6.57699 LUMO: 2.05718 factor:1 | 1 (-0.57449) | -1 | -1 |
| G: -5717.87902 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11983.24035 HOMO: -6.52529 LUMO: 1.89663 factor:1 | 1 (-0.99564) | -1 | -1 |
| G: -5717.87902 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11983.11110 HOMO: -6.30760 LUMO: 1.88031 factor:1 | 1 (-0.86638) | -1 | -1 |
| G: -5717.87902 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.92978 HOMO: -6.14977 LUMO: 1.92657 factor:1 | -1 (1.31494) | -1 | -1 |
| G: -5717.87902 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.87748 HOMO: -6.20964 LUMO: 1.83949 factor:1 | -1 (1.36724) | -1 | -1 |
| G: -5717.87902 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.71111 HOMO: -6.31848 LUMO: 1.91296 factor:1 | -1 (1.53361) | -1 | -1 |
| G: -5717.87902 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.61315 HOMO: -5.80691 LUMO: 2.19868 factor:1 | -1 (1.63157) | -1 | -1 |
| G: -5717.87902 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.15103 HOMO: -6.00827 LUMO: 2.15514 factor:1 | -1 (0.09369) | -1 | -1 |
| G: -5717.87902 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.60309 HOMO: -6.51713 LUMO: 2.08711 factor:1 | 1 (-0.35837) | -1 | -1 |
| G: -5717.87902 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.79287 HOMO: -6.32937 LUMO: 2.11705 factor:1 | -1 (0.45185) | -1 | -1 |
| G: -5717.87902 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.73547 HOMO: -6.26678 LUMO: 1.95922 factor:1 | 1 (-0.49076) | -1 | -1 |
| G: -5717.87902 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.88103 HOMO: -6.43005 LUMO: 2.56603 factor:1 | -1 (0.36368) | -1 | -1 |
| G: -5717.87902 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.84154 HOMO: -6.41644 LUMO: 2.68304 factor:1 | 1 (-0.59683) | -1 | -1 |
| G: -5717.87902 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.01437 HOMO: -5.97834 LUMO: 2.02997 factor:1 | -1 (0.23034) | -1 | -1 |
| G: -5717.87902 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.97032 HOMO: -6.14161 LUMO: 1.77690 factor:1 | -1 (1.27439) | -1 | -1 |
| G: -5717.87902 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.91770 HOMO: -6.21508 LUMO: 1.80411 factor:1 | -1 (1.32702) | -1 | -1 |
| G: -5717.87902 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.10614 HOMO: -6.46270 LUMO: 2.34562 factor:1 | -1 (1.13858) | -1 | -1 |
| G: -5717.87902 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.53315 HOMO: -6.39195 LUMO: -0.75920 factor:1 | -1 (1.71157) | -1 | -1 |
| G: -5717.87902 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.76605 HOMO: -7.08584 LUMO: -1.14016 factor:1 | -1 (1.47867) | -1 | -1 |
| G: -5717.87902 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.27266 HOMO: -6.70216 LUMO: -0.65035 factor:1 | 1 (-0.02795) | -1 | -1 |
| G: -5717.87902 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.77137 HOMO: -6.79468 LUMO: -0.83811 factor:1 | -1 (0.47334) | -1 | -1 |
| G: -5717.87902 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.90055 HOMO: -6.99877 LUMO: -0.79729 factor:1 | -1 (0.34417) | -1 | -1 |
| G: -5717.87902 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.69262 HOMO: -7.08040 LUMO: -0.85444 factor:1 | -1 (0.55209) | -1 | -1 |
| G: -5717.87902 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.45055 HOMO: -7.39333 LUMO: 0.12789 factor:1 | -1 (0.79416) | 1 | 1 |
| G: -5717.87902 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.49305 HOMO: -7.05047 LUMO: 0.13878 factor:1 | -1 (0.75166) | -1 | -1 |
| G: -5717.87902 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.52805 HOMO: -6.90897 LUMO: -0.77552 factor:1 | -1 (0.71667) | -1 | -1 |
| G: -5717.87902 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.06945 HOMO: -7.25456 LUMO: 0.05170 factor:1 | -1 (0.17527) | 1 | 1 |
| G: -5717.87902 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.83420 HOMO: -6.84638 LUMO: -0.84355 factor:1 | 1 (-0.58948) | -1 | -1 |
| G: -5717.87902 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11983.24487 HOMO: -6.78108 LUMO: -0.81634 factor:1 | 1 (-1.00015) | -1 | -1 |
| G: -5717.87902 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.23424 HOMO: -6.74570 LUMO: -0.77280 factor:1 | -1 (0.01048) | -1 | -1 |
| G: -5717.87902 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11983.17548 HOMO: -7.28177 LUMO: -1.68438 factor:1 | 1 (-0.93077) | -1 | -1 |
| G: -5717.87902 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.46156 HOMO: -7.22190 LUMO: -1.63540 factor:1 | 1 (-0.21685) | -1 | -1 |
| G: -5717.87902 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.86310 HOMO: -7.15932 LUMO: -1.57554 factor:1 | -1 (0.38161) | -1 | -1 |
| G: -5717.87902 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.56981 HOMO: -6.57971 LUMO: -0.93063 factor:1 | 1 (-0.32509) | -1 | -1 |
| G: -5717.87902 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.83292 HOMO: -6.88176 LUMO: 0.58232 factor:1 | -1 (0.41179) | -1 | -1 |
| G: -5717.87902 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.71476 HOMO: -6.85727 LUMO: 0.51430 factor:1 | 1 (-0.47005) | -1 | -1 |
| G: -5717.87902 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.96637 HOMO: -6.83550 LUMO: 0.87893 factor:1 | -1 (0.27835) | -1 | -1 |
| G: -5717.87902 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.16330 HOMO: -7.06680 LUMO: 0.87621 factor:1 | -1 (0.08142) | 1 | 1 |
| G: -5717.87902 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.29010 HOMO: -6.52257 LUMO: 0.81362 factor:1 | 1 (-0.04539) | -1 | -1 |
| G: -5717.87902 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.61077 HOMO: -6.95523 LUMO: 1.17009 factor:1 | -1 (0.63394) | -1 | -1 |
| G: -5717.87902 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.93422 HOMO: -7.21374 LUMO: 0.97145 factor:1 | 1 (-0.68951) | 1 | 1 |
| G: -5717.87902 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.99883 HOMO: -6.81373 LUMO: -1.54561 factor:1 | -1 (0.24588) | -1 | -1 |
| G: -5717.87902 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.07168 HOMO: -6.86543 LUMO: -1.52656 factor:1 | -1 (0.17304) | -1 | -1 |
| G: -5717.87902 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.11581 HOMO: -6.90081 LUMO: -0.78097 factor:1 | -1 (0.12890) | -1 | -1 |
| G: -5717.87902 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.92156 HOMO: -6.64502 LUMO: -0.82723 factor:1 | -1 (1.32315) | -1 | -1 |
| G: -5717.87902 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.88586 HOMO: -6.65591 LUMO: -0.82178 factor:1 | -1 (1.35885) | -1 | -1 |
| G: -5717.87902 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.99762 HOMO: -6.79468 LUMO: -1.46397 factor:1 | -1 (1.24710) | -1 | -1 |
| G: -5717.87902 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.49267 HOMO: -7.25728 LUMO: 0.73743 factor:1 | 1 (-0.24795) | 1 | -1 |
| G: -5717.87902 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.67140 HOMO: -7.00149 LUMO: 1.30070 factor:1 | -1 (0.57332) | -1 | -1 |
| G: -5717.87902 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.54593 HOMO: -7.07768 LUMO: 0.78097 factor:1 | -1 (0.69879) | 1 | -1 |
| G: -5717.87902 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.85500 HOMO: -6.86271 LUMO: 0.86260 factor:1 | -1 (1.38971) | -1 | -1 |
| G: -5717.87902 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.62950 HOMO: -6.94707 LUMO: 0.39729 factor:1 | -1 (1.61521) | -1 | -1 |
| G: -5717.87902 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.83593 HOMO: -6.79740 LUMO: 0.67484 factor:1 | -1 (1.40879) | -1 | -1 |
| G: -5717.87902 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.64104 HOMO: -6.91986 LUMO: -1.14288 factor:1 | -1 (1.60368) | -1 | -1 |
| G: -5717.87902 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.45273 HOMO: -6.31576 LUMO: 1.01771 factor:1 | -1 (0.79199) | -1 | -1 |
| G: -5717.87902 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.49270 HOMO: -6.81645 LUMO: 0.81362 factor:1 | -1 (0.75201) | -1 | -1 |
| G: -5717.87902 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.58546 HOMO: -6.92258 LUMO: -0.99594 factor:1 | -1 (0.65925) | -1 | -1 |
| G: -5717.87902 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.79186 HOMO: -6.81373 LUMO: 0.61770 factor:1 | -1 (0.45285) | -1 | -1 |
| G: -5717.87902 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.55531 HOMO: -7.18653 LUMO: 1.19186 factor:1 | -1 (0.68940) | 1 | 1 |
| G: -5717.87902 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.11851 HOMO: -7.00693 LUMO: 0.45715 factor:1 | -1 (0.12621) | -1 | -1 |
| G: -5717.87902 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.64916 HOMO: -7.11306 LUMO: 0.53334 factor:1 | 1 (-0.40444) | 1 | 1 |
| G: -5717.87902 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.91742 HOMO: -6.63414 LUMO: -1.64357 factor:1 | -1 (0.32730) | -1 | -1 |
| G: -5717.87902 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.51729 HOMO: -6.22052 LUMO: -0.74015 factor:1 | 1 (-0.27258) | -1 | -1 |
| G: -5717.87902 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.80854 HOMO: -6.81101 LUMO: -0.50069 factor:1 | -1 (0.43617) | -1 | -1 |
| G: -5717.87902 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.59177 HOMO: -6.71849 LUMO: -0.51974 factor:1 | 1 (-0.34705) | -1 | -1 |
| G: -5717.87902 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.94561 HOMO: -6.72121 LUMO: -1.77690 factor:1 | -1 (0.29911) | -1 | -1 |
| G: -5717.87902 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.82370 HOMO: -6.94162 LUMO: -1.78779 factor:1 | -1 (0.42101) | -1 | -1 |
| G: -5717.87902 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.94590 HOMO: -6.91169 LUMO: 0.88981 factor:1 | 1 (-0.70118) | -1 | -1 |
| G: -5717.87902 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.43783 HOMO: -6.97428 LUMO: 0.70750 factor:1 | 1 (-0.19312) | -1 | -1 |
| G: -5717.87902 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.54877 HOMO: -6.74842 LUMO: 1.15921 factor:1 | 1 (-0.30406) | -1 | -1 |
| G: -5717.87902 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.48132 HOMO: -7.25183 LUMO: -0.99594 factor:1 | 1 (-0.23660) | -1 | -1 |
| G: -5717.87902 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11983.08628 HOMO: -6.43821 LUMO: -1.00410 factor:1 | 1 (-0.84157) | -1 | -1 |
| G: -5717.87902 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.06531 HOMO: -6.52257 LUMO: -0.68573 factor:1 | -1 (0.17940) | -1 | -1 |
| G: -5717.87902 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.20605 HOMO: -6.60148 LUMO: -0.52518 factor:1 | -1 (0.03867) | -1 | -1 |
| G: -5717.87902 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.63809 HOMO: -6.07086 LUMO: -1.39594 factor:1 | -1 (0.60662) | -1 | -1 |
| G: -5717.87902 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.43528 HOMO: -6.78108 LUMO: -1.54833 factor:1 | -1 (0.80943) | -1 | -1 |
| G: -5717.87902 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.32308 HOMO: -6.73482 LUMO: -1.01498 factor:1 | 1 (-0.07837) | -1 | -1 |
| G: -5717.87902 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.19202 HOMO: -6.85183 LUMO: 1.06669 factor:1 | -1 (1.05270) | -1 | -1 |
| G: -5717.87902 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.24617 HOMO: -6.98516 LUMO: 1.43948 factor:1 | -1 (0.99855) | -1 | -1 |
| G: -5717.87902 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.53770 HOMO: -6.94162 LUMO: 0.79185 factor:1 | 1 (-0.29298) | -1 | -1 |
| G: -5717.87902 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.22293 HOMO: -6.67495 LUMO: -1.06669 factor:1 | -1 (1.02179) | -1 | -1 |
| G: -5717.87902 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.23533 HOMO: -6.88720 LUMO: -1.00682 factor:1 | -1 (0.00939) | -1 | -1 |
| G: -5717.87902 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.16564 HOMO: -6.85999 LUMO: -0.78097 factor:1 | -1 (0.07908) | -1 | -1 |
| G: -5717.87902 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.70157 HOMO: -6.51713 LUMO: -0.89798 factor:1 | 1 (-0.45685) | -1 | -1 |
| G: -5717.87902 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.87978 HOMO: -6.63141 LUMO: -0.91430 factor:1 | -1 (0.36493) | -1 | -1 |
| G: -5717.87902 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.30004 HOMO: -6.63414 LUMO: 0.04354 factor:1 | 1 (-0.05532) | -1 | -1 |
| G: -5717.87902 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.83361 HOMO: -6.65046 LUMO: -0.73743 factor:1 | -1 (0.41111) | -1 | -1 |
| G: -5717.87902 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.35021 HOMO: -6.73754 LUMO: -0.71838 factor:1 | 1 (-0.10550) | -1 | -1 |
| G: -5717.87902 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.52009 HOMO: -6.65863 LUMO: -0.60137 factor:1 | 1 (-0.27538) | -1 | -1 |
| G: -5717.87902 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.76838 HOMO: -6.61509 LUMO: -0.47892 factor:1 | -1 (0.47634) | -1 | -1 |
| G: -5717.87902 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.29233 HOMO: -6.82189 LUMO: -0.64763 factor:1 | 1 (-0.04762) | -1 | -1 |
| G: -5717.87902 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.49846 HOMO: -6.56883 LUMO: -0.51974 factor:1 | 1 (-0.25375) | -1 | -1 |
| G: -5717.87902 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.27277 HOMO: -6.97428 LUMO: -0.95512 factor:1 | 1 (-0.02805) | -1 | -1 |
| G: -5717.87902 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.13464 HOMO: -6.70489 LUMO: -0.04082 factor:1 | -1 (0.11007) | -1 | -1 |
| G: -5717.87902 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.04751 HOMO: -6.74026 LUMO: 0.02177 factor:1 | -1 (0.19720) | -1 | -1 |
| G: -5717.87902 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.92789 HOMO: -6.50080 LUMO: -0.89525 factor:1 | -1 (0.31682) | -1 | -1 |
| G: -5717.87902 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.61254 HOMO: -6.46815 LUMO: -0.61226 factor:1 | -1 (0.63217) | -1 | -1 |
| G: -5717.87902 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.17277 HOMO: -6.57971 LUMO: -0.64219 factor:1 | -1 (0.07195) | -1 | -1 |
| G: -5717.87902 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.10449 HOMO: -7.17836 LUMO: 0.37280 factor:1 | -1 (0.14022) | 1 | 1 |
| G: -5717.87902 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.26578 HOMO: -6.67223 LUMO: 0.12245 factor:1 | 1 (-0.02106) | -1 | -1 |
| G: -5717.87902 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.93731 HOMO: -6.55250 LUMO: 0.22858 factor:1 | -1 (0.30741) | -1 | -1 |
| G: -5717.87902 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.36864 HOMO: -6.97156 LUMO: -1.12927 factor:1 | 1 (-0.12392) | -1 | -1 |
| G: -5717.87902 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.32970 HOMO: -6.78924 LUMO: -0.84900 factor:1 | 1 (-0.08498) | -1 | -1 |
| G: -5717.87902 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.19758 HOMO: -6.65046 LUMO: -0.65307 factor:1 | -1 (0.04713) | -1 | -1 |
| G: -5717.87902 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.89891 HOMO: -7.41782 LUMO: 0.08980 factor:1 | -1 (0.34580) | 1 | 1 |
| G: -5717.87902 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.00512 HOMO: -6.56339 LUMO: -0.68573 factor:1 | -1 (0.23960) | -1 | -1 |
| G: -5717.87902 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.82694 HOMO: -6.31032 LUMO: -0.31837 factor:1 | -1 (0.41778) | -1 | -1 |
| G: -5717.87902 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.55836 HOMO: -6.72938 LUMO: -0.45987 factor:1 | -1 (0.68635) | -1 | -1 |
| G: -5717.87902 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.59083 HOMO: -6.59876 LUMO: -1.03131 factor:1 | -1 (0.65389) | -1 | -1 |
| G: -5717.87902 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.95303 HOMO: -7.29265 LUMO: 0.29660 factor:1 | 1 (-0.70831) | 1 | 1 |
| G: -5717.87902 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.00272 HOMO: -6.42189 LUMO: -0.51157 factor:1 | -1 (0.24199) | -1 | -1 |
| G: -5717.87902 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.29906 HOMO: -6.27767 LUMO: -0.52790 factor:1 | 1 (-0.05434) | -1 | -1 |
| G: -5717.87902 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.00466 HOMO: -6.41644 LUMO: -0.44627 factor:1 | -1 (1.24005) | -1 | -1 |
| G: -5717.87902 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.99627 HOMO: -6.23413 LUMO: -0.52790 factor:1 | -1 (0.24844) | -1 | -1 |
| G: -5717.87902 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.01852 HOMO: -6.63414 LUMO: -0.44082 factor:1 | -1 (1.22620) | -1 | -1 |
| G: -5717.87902 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.96186 HOMO: -7.03142 LUMO: 0.47076 factor:1 | -1 (1.28285) | -1 | -1 |
| G: -5717.87902 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.93759 HOMO: -6.62053 LUMO: -0.14422 factor:1 | -1 (1.30713) | -1 | -1 |
| G: -5717.87902 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.11566 HOMO: -6.22324 LUMO: 1.96194 factor:1 | -1 (1.12905) | -1 | -1 |
| G: -5717.87902 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.08208 HOMO: -6.17971 LUMO: 1.71704 factor:1 | -1 (1.16263) | -1 | -1 |
| G: -5717.87902 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.19392 HOMO: -6.70761 LUMO: 1.68711 factor:1 | -1 (1.05079) | -1 | -1 |
| G: -5717.87902 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.06780 HOMO: -6.52801 LUMO: 1.56193 factor:1 | -1 (1.17692) | -1 | -1 |
| G: -5717.87902 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.00134 HOMO: -6.55794 LUMO: 1.52384 factor:1 | -1 (0.24338) | -1 | -1 |
| G: -5717.87902 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.64519 HOMO: -6.47359 LUMO: 1.82316 factor:1 | -1 (0.59952) | -1 | -1 |
| G: -5717.87902 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.95146 HOMO: -6.65863 LUMO: 1.83133 factor:1 | -1 (0.29326) | -1 | -1 |
| G: -5717.87902 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.06331 HOMO: -6.46270 LUMO: 1.90208 factor:1 | -1 (1.18141) | -1 | -1 |
| G: -5717.87902 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.28478 HOMO: -6.41917 LUMO: 2.03269 factor:1 | -1 (0.95994) | -1 | -1 |
| G: -5717.87902 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.94080 HOMO: -6.48992 LUMO: 1.87486 factor:1 | -1 (1.30392) | -1 | -1 |
| G: -5717.87902 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.00856 HOMO: -6.51985 LUMO: 1.69527 factor:1 | -1 (1.23616) | -1 | -1 |
| G: -5717.87902 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.94804 HOMO: -6.36202 LUMO: 2.05718 factor:1 | -1 (1.29668) | -1 | -1 |
| G: -5717.87902 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.83119 HOMO: -5.96474 LUMO: 1.88575 factor:1 | -1 (1.41352) | -1 | -1 |
| G: -5717.87902 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.30112 HOMO: -6.56339 LUMO: 2.04630 factor:1 | 1 (-0.05641) | -1 | -1 |
| G: -5717.87902 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.90673 HOMO: -6.43277 LUMO: 1.98371 factor:1 | -1 (1.33798) | -1 | -1 |
| G: -5717.87902 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.88933 HOMO: -6.53345 LUMO: 2.06262 factor:1 | -1 (0.35538) | -1 | -1 |
| G: -5717.87902 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11983.04617 HOMO: -5.81779 LUMO: 2.11432 factor:1 | 1 (-0.80146) | -1 | -1 |
| G: -5717.87902 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11983.41562 HOMO: -5.91848 LUMO: 1.86942 factor:1 | 1 (-1.17091) | -1 | -1 |
| G: -5717.87902 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11983.09200 HOMO: -6.48447 LUMO: 1.70343 factor:1 | 1 (-0.84728) | -1 | -1 |
| G: -5717.87902 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11983.60504 HOMO: -6.29671 LUMO: -0.89525 factor:1 | 1 (-1.36032) | -1 | -1 |
| G: -5717.87902 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11983.24283 HOMO: -6.63414 LUMO: -0.76192 factor:1 | 1 (-0.99811) | -1 | -1 |
| G: -5717.87902 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11983.48305 HOMO: -6.56883 LUMO: -0.86260 factor:1 | 1 (-1.23834) | -1 | -1 |
| G: -5717.87902 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.35066 HOMO: -6.93074 LUMO: -0.27483 factor:1 | -1 (0.89406) | -1 | -1 |
| G: -5717.87902 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.20358 HOMO: -6.85999 LUMO: -0.01905 factor:1 | -1 (1.04113) | -1 | -1 |
| G: -5717.87902 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.55765 HOMO: -6.26406 LUMO: 0.21769 factor:1 | -1 (0.68706) | -1 | -1 |
| G: -5717.87902 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.79080 HOMO: -6.62325 LUMO: 0.31293 factor:1 | -1 (0.45391) | -1 | -1 |
| G: -5717.87902 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.09943 HOMO: -6.59604 LUMO: 0.19592 factor:1 | -1 (0.14528) | -1 | -1 |
| G: -5717.87902 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.25669 HOMO: -6.43277 LUMO: -0.27756 factor:1 | 1 (-0.01197) | -1 | -1 |
| G: -5717.87902 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.93170 HOMO: -6.54978 LUMO: -0.46531 factor:1 | -1 (0.31301) | -1 | -1 |
| G: -5717.87902 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.72492 HOMO: -6.65046 LUMO: -0.15783 factor:1 | -1 (0.51979) | -1 | -1 |
| G: -5717.87902 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.18697 HOMO: -7.28721 LUMO: 0.23946 factor:1 | -1 (0.05774) | 1 | 1 |
| G: -5717.87902 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11983.32218 HOMO: -6.71849 LUMO: -0.56600 factor:1 | 1 (-1.07746) | -1 | -1 |
| G: -5717.87902 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.41626 HOMO: -6.85183 LUMO: -0.84355 factor:1 | 1 (-0.17154) | -1 | -1 |
| G: -5717.87902 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.86078 HOMO: -6.53345 LUMO: -0.84627 factor:1 | 1 (-0.61607) | -1 | -1 |
| G: -5717.87902 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11983.07698 HOMO: -6.60148 LUMO: -0.63130 factor:1 | 1 (-0.83226) | -1 | -1 |
| G: -5717.87902 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.42560 HOMO: -6.36202 LUMO: -0.60137 factor:1 | -1 (0.81912) | -1 | -1 |
| G: -5717.87902 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.33996 HOMO: -6.28855 LUMO: -0.52790 factor:1 | -1 (0.90475) | -1 | -1 |
| G: -5717.87902 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.39813 HOMO: -7.07224 LUMO: 0.41906 factor:1 | 1 (-0.15342) | 1 | 1 |
| G: -5717.87902 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.50265 HOMO: -6.36202 LUMO: -0.24218 factor:1 | 1 (-0.25794) | -1 | -1 |
| G: -5717.87902 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.41049 HOMO: -6.43549 LUMO: 0.14150 factor:1 | 1 (-0.16577) | -1 | -1 |
| G: -5717.87902 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.87393 HOMO: -6.76747 LUMO: -0.40545 factor:1 | -1 (0.37078) | -1 | -1 |
| G: -5717.87902 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.09211 HOMO: -6.15249 LUMO: -0.51157 factor:1 | -1 (0.15260) | -1 | -1 |
| G: -5717.87902 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.26921 HOMO: -6.33753 LUMO: -0.02993 factor:1 | 1 (-0.02449) | -1 | -1 |
| G: -5717.87902 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.39223 HOMO: -6.49808 LUMO: -0.83811 factor:1 | 1 (-0.14751) | -1 | -1 |
| G: -5717.87902 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.03946 HOMO: -6.64502 LUMO: -0.46259 factor:1 | -1 (0.20526) | -1 | -1 |
| G: -5717.87902 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.44279 HOMO: -6.34570 LUMO: 0.22041 factor:1 | 1 (-0.19807) | -1 | -1 |
| G: -5717.87902 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.08643 HOMO: -6.63414 LUMO: -0.13606 factor:1 | -1 (0.15829) | -1 | -1 |
| G: -5717.87902 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.60595 HOMO: -6.59604 LUMO: -0.79729 factor:1 | -1 (0.63876) | -1 | -1 |
| G: -5717.87902 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.50481 HOMO: -7.09401 LUMO: 0.31837 factor:1 | -1 (0.73990) | 1 | 1 |
| G: -5717.87902 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.94147 HOMO: -6.48719 LUMO: -0.31021 factor:1 | -1 (0.30324) | -1 | -1 |
| G: -5717.87902 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.31688 HOMO: -7.11306 LUMO: 0.39729 factor:1 | 1 (-0.07216) | 1 | 1 |
| G: -5717.87902 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.04262 HOMO: -6.95251 LUMO: 0.41089 factor:1 | -1 (0.20210) | -1 | -1 |
| G: -5717.87902 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.23541 HOMO: -6.61509 LUMO: -0.41906 factor:1 | -1 (0.00931) | -1 | -1 |
| G: -5717.87902 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.00321 HOMO: -6.25318 LUMO: -0.47348 factor:1 | -1 (0.24150) | -1 | -1 |
| G: -5717.87902 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.86555 HOMO: -6.77019 LUMO: -0.10340 factor:1 | -1 (0.37916) | -1 | -1 |
| G: -5717.87902 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.35898 HOMO: -6.54706 LUMO: -0.46259 factor:1 | -1 (0.88573) | -1 | -1 |
| G: -5717.87902 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.39326 HOMO: -6.34297 LUMO: -0.50341 factor:1 | 1 (-0.14855) | -1 | -1 |
| G: -5717.87902 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.79524 HOMO: -6.20692 LUMO: -0.51974 factor:1 | -1 (0.44948) | -1 | -1 |
| G: -5717.87902 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.25672 HOMO: -7.03686 LUMO: 0.46804 factor:1 | 1 (-0.01200) | -1 | -1 |
| G: -5717.87902 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.22218 HOMO: -6.47087 LUMO: 0.22585 factor:1 | -1 (0.02253) | -1 | -1 |
| G: -5717.87902 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.19141 HOMO: -6.41917 LUMO: 0.19320 factor:1 | -1 (0.05331) | -1 | -1 |
| G: -5717.87902 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.35860 HOMO: -6.61237 LUMO: -0.04354 factor:1 | -1 (0.88611) | -1 | -1 |
| G: -5717.87902 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.42045 HOMO: -6.56339 LUMO: 0.36735 factor:1 | 1 (-0.17573) | -1 | -1 |
| G: -5717.87902 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.40605 HOMO: -6.54978 LUMO: 1.12655 factor:1 | 1 (-0.16134) | -1 | -1 |
| G: -5717.87902 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.13005 HOMO: -6.43277 LUMO: 1.17553 factor:1 | -1 (0.11467) | -1 | -1 |
| G: -5717.87902 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.55547 HOMO: -6.29944 LUMO: 1.40955 factor:1 | 1 (-0.31075) | -1 | -1 |
| G: -5717.87902 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.95361 HOMO: -6.74842 LUMO: 0.74015 factor:1 | -1 (0.29111) | -1 | -1 |
| G: -5717.87902 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.60049 HOMO: -6.15522 LUMO: 1.94289 factor:1 | -1 (0.64423) | -1 | -1 |
| G: -5717.87902 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.40132 HOMO: -6.20147 LUMO: 1.40139 factor:1 | 1 (-0.15660) | -1 | -1 |
| G: -5717.87902 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.34523 HOMO: -6.41100 LUMO: 1.40139 factor:1 | 1 (-0.10052) | -1 | -1 |
| G: -5717.87902 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.11913 HOMO: -6.74570 LUMO: 1.80956 factor:1 | -1 (0.12558) | -1 | -1 |
| G: -5717.87902 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.32942 HOMO: -6.60148 LUMO: -1.04764 factor:1 | 1 (-0.08471) | -1 | -1 |
| G: -5717.87902 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.29217 HOMO: -6.82734 LUMO: -0.83267 factor:1 | 1 (-0.04746) | -1 | -1 |
| G: -5717.87902 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.46582 HOMO: -7.01782 LUMO: -0.32382 factor:1 | -1 (0.77890) | -1 | -1 |
| G: -5717.87902 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.36666 HOMO: -6.54434 LUMO: 0.11157 factor:1 | -1 (0.87806) | -1 | -1 |
| G: -5717.87902 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.42072 HOMO: -6.53617 LUMO: 0.32926 factor:1 | 1 (-0.17600) | -1 | -1 |
| G: -5717.87902 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.18882 HOMO: -6.62597 LUMO: -0.60137 factor:1 | -1 (0.05589) | -1 | -1 |
| G: -5717.87902 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.26221 HOMO: -6.60965 LUMO: -0.75376 factor:1 | 1 (-0.01750) | -1 | -1 |
| G: -5717.87902 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.89932 HOMO: -6.29399 LUMO: 0.06803 factor:1 | -1 (0.34539) | -1 | -1 |
| G: -5717.87902 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.94106 HOMO: -6.60692 LUMO: -0.47076 factor:1 | -1 (0.30365) | -1 | -1 |
| G: -5717.87902 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.64429 HOMO: -7.33891 LUMO: 0.39184 factor:1 | 1 (-0.39957) | 1 | 1 |
| G: -5717.87902 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.93931 HOMO: -6.60692 LUMO: 1.46125 factor:1 | 1 (-0.69460) | -1 | -1 |
| G: -5717.87902 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.78456 HOMO: -6.21780 LUMO: 2.09256 factor:1 | 1 (-0.53985) | -1 | -1 |
| G: -5717.87902 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11983.28261 HOMO: -6.28311 LUMO: 1.80411 factor:1 | 1 (-1.03790) | -1 | -1 |
| G: -5717.87902 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.90976 HOMO: -6.51168 LUMO: 1.84765 factor:1 | 1 (-0.66505) | -1 | -1 |
| G: -5717.87902 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11983.29409 HOMO: -6.66951 LUMO: 2.01636 factor:1 | 1 (-1.04938) | -1 | -1 |
| G: -5717.87902 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11983.47143 HOMO: -6.75387 LUMO: 1.73881 factor:1 | 1 (-1.22672) | -1 | -1 |
| G: -5717.87902 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11983.78221 HOMO: -6.77291 LUMO: 1.89935 factor:1 | 1 (-1.53750) | -1 | -1 |
| G: -5717.87902 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11983.05172 HOMO: -6.36474 LUMO: 1.61091 factor:1 | 1 (-0.80701) | -1 | -1 |
| G: -5717.87902 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11983.22778 HOMO: -6.60420 LUMO: 1.40955 factor:1 | 1 (-0.98307) | -1 | -1 |
| G: -5717.87902 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11983.18998 HOMO: -6.81645 LUMO: 1.59731 factor:1 | 1 (-0.94527) | -1 | -1 |
| G: -5717.87902 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.52299 HOMO: -5.90215 LUMO: 2.12249 factor:1 | -1 (0.72173) | -1 | -1 |
| G: -5717.87902 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.25413 HOMO: -6.26950 LUMO: 1.62996 factor:1 | 1 (-0.00942) | -1 | -1 |
| G: -5717.87902 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.19625 HOMO: -6.41100 LUMO: 1.80684 factor:1 | -1 (0.04846) | -1 | -1 |
| G: -5717.87902 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.32295 HOMO: -6.64230 LUMO: 2.23405 factor:1 | 1 (-0.07823) | -1 | -1 |
| G: -5717.87902 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.27122 HOMO: -6.66951 LUMO: 2.21501 factor:1 | 1 (-0.02650) | -1 | -1 |
| G: -5717.87902 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.67419 HOMO: -6.90897 LUMO: 2.00004 factor:1 | 1 (-0.42948) | -1 | -1 |
| G: -5717.87902 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.04286 HOMO: -6.61781 LUMO: 1.42043 factor:1 | -1 (0.20185) | -1 | -1 |
| G: -5717.87902 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.62450 HOMO: -6.56611 LUMO: 1.60003 factor:1 | 1 (-0.37979) | -1 | -1 |
| G: -5717.87902 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.20997 HOMO: -6.70489 LUMO: 1.78779 factor:1 | -1 (0.03475) | -1 | -1 |
| G: -5717.87902 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.14798 HOMO: -6.46815 LUMO: 1.59459 factor:1 | -1 (0.09674) | -1 | -1 |
| G: -5717.87902 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.20151 HOMO: -6.31304 LUMO: 1.36873 factor:1 | -1 (1.04320) | -1 | -1 |
| G: -5717.87902 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.50639 HOMO: -6.22597 LUMO: 1.54833 factor:1 | -1 (0.73833) | -1 | -1 |
| G: -5717.87902 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.18700 HOMO: -5.63004 LUMO: 1.96466 factor:1 | -1 (0.05772) | -1 | -1 |
| G: -5717.87902 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.15125 HOMO: -7.02598 LUMO: 1.79323 factor:1 | -1 (1.09346) | -1 | -1 |
| G: -5717.87902 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.12145 HOMO: -6.78924 LUMO: 2.10888 factor:1 | -1 (0.12327) | -1 | -1 |
| G: -5717.87902 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.30069 HOMO: -6.13345 LUMO: 2.07351 factor:1 | 1 (-0.05597) | -1 | -1 |
| G: -5717.87902 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.60921 HOMO: -6.46270 LUMO: -0.37552 factor:1 | 1 (-0.36450) | -1 | -1 |
| G: -5717.87902 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.69344 HOMO: -6.51985 LUMO: -0.49525 factor:1 | -1 (0.55128) | -1 | -1 |
| G: -5717.87902 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.08409 HOMO: -6.60965 LUMO: 1.90480 factor:1 | -1 (0.16063) | -1 | -1 |
| G: -5717.87902 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.70356 HOMO: -6.51168 LUMO: 1.92112 factor:1 | -1 (0.54115) | -1 | -1 |
| G: -5717.87902 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.58135 HOMO: -6.71305 LUMO: 1.91024 factor:1 | 1 (-0.33663) | -1 | -1 |
| G: -5717.87902 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.12656 HOMO: -6.86815 LUMO: 2.02997 factor:1 | -1 (0.11815) | -1 | -1 |
| G: -5717.87902 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.23881 HOMO: -6.69944 LUMO: 1.95106 factor:1 | -1 (0.00590) | -1 | -1 |
| G: -5717.87902 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.04087 HOMO: -6.45182 LUMO: 1.66806 factor:1 | -1 (0.20384) | -1 | -1 |
| G: -5717.87902 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.75678 HOMO: -6.44638 LUMO: 2.16058 factor:1 | 1 (-0.51206) | -1 | -1 |
| G: -5717.87902 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.80735 HOMO: -6.65591 LUMO: 1.95106 factor:1 | -1 (0.43737) | -1 | -1 |
| G: -5717.87902 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.68148 HOMO: -6.35114 LUMO: 1.42316 factor:1 | 1 (-0.43677) | -1 | -1 |
| G: -5717.87902 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.28042 HOMO: -6.48719 LUMO: 1.59187 factor:1 | 1 (-0.03570) | -1 | -1 |
| G: -5717.87902 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.26287 HOMO: -7.05591 LUMO: 1.61908 factor:1 | -1 (0.98184) | -1 | -1 |
| G: -5717.87902 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.31119 HOMO: -6.92258 LUMO: 1.87214 factor:1 | 1 (-0.06648) | -1 | -1 |
| G: -5717.87902 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11983.63650 HOMO: -5.85861 LUMO: 2.11705 factor:1 | 1 (-1.39178) | -1 | -1 |
| G: -5717.87902 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11983.66539 HOMO: -6.27767 LUMO: 1.75513 factor:1 | 1 (-1.42068) | -1 | -1 |
| G: -5717.87902 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.70127 HOMO: -6.16882 LUMO: 1.73881 factor:1 | 1 (-0.45655) | -1 | -1 |
| G: -5717.87902 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11983.62490 HOMO: -6.62053 LUMO: 1.39594 factor:1 | 1 (-1.38019) | -1 | -1 |
| G: -5717.87902 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11983.51660 HOMO: -5.46405 LUMO: 1.68166 factor:1 | 1 (-1.27189) | -1 | -1 |
| G: -5717.87902 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.17960 HOMO: -6.39740 LUMO: 1.68711 factor:1 | -1 (0.06512) | -1 | -1 |
| G: -5717.87902 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.09726 HOMO: -6.99333 LUMO: 2.08439 factor:1 | -1 (0.14746) | -1 | -1 |
| G: -5717.87902 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.11894 HOMO: -6.16882 LUMO: 1.71976 factor:1 | -1 (0.12577) | -1 | -1 |
| G: -5717.87902 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.88234 HOMO: -7.19741 LUMO: 2.24766 factor:1 | -1 (0.36237) | 1 | 1 |
| G: -5717.87902 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.61286 HOMO: -6.77291 LUMO: 2.17691 factor:1 | 1 (-0.36814) | -1 | -1 |
| G: -5717.87902 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.95513 HOMO: -6.29944 LUMO: 2.16603 factor:1 | -1 (0.28958) | -1 | -1 |
| G: -5717.87902 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.78525 HOMO: -6.10079 LUMO: 1.83949 factor:1 | -1 (0.45946) | -1 | -1 |
| G: -5717.87902 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.82220 HOMO: -6.63686 LUMO: 2.05990 factor:1 | -1 (0.42251) | -1 | -1 |
| G: -5717.87902 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.56197 HOMO: -6.91713 LUMO: 1.87486 factor:1 | 1 (-0.31726) | -1 | -1 |
| G: -5717.87902 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.15421 HOMO: -6.63958 LUMO: 1.79323 factor:1 | -1 (0.09051) | -1 | -1 |
| G: -5717.87902 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.22012 HOMO: -6.61781 LUMO: 1.70071 factor:1 | -1 (1.02459) | -1 | -1 |
| G: -5717.87902 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.20137 HOMO: -6.20420 LUMO: 1.82861 factor:1 | -1 (0.04335) | -1 | -1 |
| G: -5717.87902 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.17451 HOMO: -6.47903 LUMO: -2.16875 factor:1 | -1 (0.07021) | -1 | -1 |
| G: -5717.87902 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11983.26414 HOMO: -6.53073 LUMO: 2.18235 factor:1 | 1 (-1.01942) | -1 | -1 |
| G: -5717.87902 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.41661 HOMO: -7.01782 LUMO: 1.72520 factor:1 | 1 (-0.17189) | -1 | -1 |
| G: -5717.87902 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.19767 HOMO: -6.66135 LUMO: -0.75648 factor:1 | -1 (0.04705) | -1 | -1 |
| G: -5717.87902 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11983.13243 HOMO: -7.56749 LUMO: 0.22585 factor:1 | 1 (-0.88772) | 1 | 1 |
| G: -5717.87902 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11983.09341 HOMO: -6.45182 LUMO: -0.71294 factor:1 | 1 (-0.84870) | -1 | -1 |
| G: -5717.87902 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.17383 HOMO: -6.31032 LUMO: -0.34286 factor:1 | -1 (0.07089) | -1 | -1 |
| G: -5717.87902 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.90629 HOMO: -6.41917 LUMO: 2.04085 factor:1 | -1 (0.33843) | -1 | -1 |
| G: -5717.87902 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11983.47010 HOMO: -6.61781 LUMO: 1.98915 factor:1 | 1 (-1.22538) | -1 | -1 |
| G: -5717.87902 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11983.22759 HOMO: -5.86405 LUMO: 1.57282 factor:1 | 1 (-0.98288) | -1 | -1 |
| G: -5717.87902 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.60578 HOMO: -6.44094 LUMO: 1.80956 factor:1 | 1 (-0.36107) | -1 | -1 |
| G: -5717.87902 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.10613 HOMO: -6.59060 LUMO: 2.08167 factor:1 | -1 (0.13859) | -1 | -1 |
| G: -5717.87902 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.01255 HOMO: -6.20147 LUMO: 1.69799 factor:1 | -1 (0.23217) | -1 | -1 |
| G: -5717.87902 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.18545 HOMO: -6.50352 LUMO: -0.41361 factor:1 | -1 (0.05927) | -1 | -1 |
| G: -5717.87902 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.80411 HOMO: -6.10896 LUMO: -0.55783 factor:1 | -1 (0.44061) | -1 | -1 |
| G: -5717.87902 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.13062 HOMO: -6.74842 LUMO: -0.56872 factor:1 | -1 (0.11410) | -1 | -1 |
| G: -5717.87902 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.91570 HOMO: -6.59060 LUMO: -0.22041 factor:1 | -1 (0.32901) | -1 | -1 |
| G: -5717.87902 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.06610 HOMO: -6.22052 LUMO: -0.60137 factor:1 | -1 (0.17862) | -1 | -1 |
| G: -5717.87902 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.77009 HOMO: -6.65863 LUMO: 0.07891 factor:1 | -1 (0.47462) | -1 | -1 |
| G: -5717.87902 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.71815 HOMO: -6.57427 LUMO: 1.71160 factor:1 | -1 (0.52657) | -1 | -1 |
| G: -5717.87902 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.22624 HOMO: -5.84773 LUMO: 1.99459 factor:1 | -1 (0.01848) | -1 | -1 |
| G: -5717.87902 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11983.18623 HOMO: -6.02188 LUMO: 1.91296 factor:1 | 1 (-0.94151) | -1 | -1 |
| G: -5717.87902 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.19002 HOMO: -6.17698 LUMO: 2.00004 factor:1 | -1 (0.05469) | -1 | -1 |
| G: -5717.87902 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.90191 HOMO: -6.02732 LUMO: 1.90752 factor:1 | -1 (1.34280) | -1 | -1 |
| G: -5717.87902 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.73285 HOMO: -6.68584 LUMO: -0.50885 factor:1 | -1 (1.51186) | -1 | -1 |
| G: -5717.87902 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.13267 HOMO: -6.61781 LUMO: -0.73471 factor:1 | -1 (1.11205) | -1 | -1 |
| G: -5717.87902 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.82746 HOMO: -6.66407 LUMO: -0.79729 factor:1 | -1 (1.41725) | -1 | -1 |
| G: -5717.87902 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.00351 HOMO: -6.56339 LUMO: 0.23130 factor:1 | -1 (0.24120) | -1 | -1 |
| G: -5717.87902 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.12243 HOMO: -6.76747 LUMO: 0.08980 factor:1 | -1 (0.12229) | -1 | -1 |
| G: -5717.87902 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.85510 HOMO: -6.70489 LUMO: -0.53334 factor:1 | -1 (0.38961) | -1 | -1 |
| G: -5717.87902 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.79520 HOMO: -7.28993 LUMO: 0.10885 factor:1 | 1 (-0.55049) | 1 | 1 |
| G: -5717.87902 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.04387 HOMO: -6.22052 LUMO: 0.51974 factor:1 | -1 (0.20085) | -1 | -1 |
| G: -5717.87902 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.29040 HOMO: -6.81645 LUMO: 0.25307 factor:1 | 1 (-0.04569) | -1 | -1 |
| G: -5717.87902 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.36527 HOMO: -6.80285 LUMO: 0.02721 factor:1 | -1 (0.87944) | -1 | -1 |
| G: -5717.87902 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.20287 HOMO: -6.51441 LUMO: 0.08163 factor:1 | -1 (1.04184) | -1 | -1 |
| G: -5717.87902 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.47960 HOMO: -6.73482 LUMO: -0.77008 factor:1 | 1 (-0.23489) | -1 | -1 |
| G: -5717.87902 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.18611 HOMO: -6.29127 LUMO: -0.44355 factor:1 | -1 (1.05860) | -1 | -1 |
| G: -5717.87902 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.19835 HOMO: -6.72938 LUMO: -0.64763 factor:1 | -1 (0.04637) | -1 | -1 |
| G: -5717.87902 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11983.45154 HOMO: -6.49264 LUMO: -0.74559 factor:1 | 1 (-1.20682) | -1 | -1 |
| G: -5717.87902 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11983.07129 HOMO: -6.67223 LUMO: -0.55239 factor:1 | 1 (-0.82657) | -1 | -1 |
| G: -5717.87902 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.40614 HOMO: -6.33481 LUMO: 0.33198 factor:1 | -1 (0.83857) | -1 | -1 |
| G: -5717.87902 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.59768 HOMO: -6.76475 LUMO: -0.25307 factor:1 | -1 (0.64703) | -1 | -1 |
| G: -5717.87902 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.59942 HOMO: -6.65318 LUMO: 0.03810 factor:1 | -1 (0.64529) | -1 | -1 |
| G: -5717.87902 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.73379 HOMO: -6.09263 LUMO: 0.21497 factor:1 | -1 (0.51092) | -1 | -1 |
| G: -5717.87902 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.74797 HOMO: -6.32120 LUMO: -0.85444 factor:1 | -1 (0.49674) | -1 | -1 |
| G: -5717.87902 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.07887 HOMO: -6.57155 LUMO: -0.67484 factor:1 | -1 (1.16584) | -1 | -1 |
| G: -5717.87902 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.31468 HOMO: -6.53345 LUMO: -0.78913 factor:1 | -1 (0.93003) | -1 | -1 |
| G: -5717.87902 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11983.40525 HOMO: -7.07768 LUMO: 0.28844 factor:1 | 1 (-1.16054) | 1 | 1 |
| G: -5717.87902 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.99025 HOMO: -6.75114 LUMO: 0.18776 factor:1 | 1 (-0.74554) | -1 | -1 |
| G: -5717.87902 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.84932 HOMO: -6.77019 LUMO: -0.12245 factor:1 | 1 (-0.60461) | -1 | -1 |
| G: -5717.87902 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.96656 HOMO: -6.43549 LUMO: 0.16327 factor:1 | -1 (0.27815) | -1 | -1 |
| G: -5717.87902 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.95285 HOMO: -6.69400 LUMO: -0.16327 factor:1 | -1 (0.29187) | -1 | -1 |
| G: -5717.87902 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.08240 HOMO: -6.38651 LUMO: -0.61770 factor:1 | -1 (0.16232) | -1 | -1 |
| G: -5717.87902 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.85845 HOMO: -6.34297 LUMO: -0.33198 factor:1 | -1 (0.38627) | -1 | -1 |
| G: -5717.87902 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.08180 HOMO: -7.51578 LUMO: 0.02177 factor:1 | -1 (0.16291) | 1 | 1 |
| G: -5717.87902 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.98593 HOMO: -6.47359 LUMO: -0.22585 factor:1 | -1 (0.25878) | -1 | -1 |
| G: -5717.87902 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.17201 HOMO: -6.68040 LUMO: -0.47076 factor:1 | -1 (0.07271) | -1 | -1 |
| G: -5717.87902 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.96768 HOMO: -6.75659 LUMO: -0.57688 factor:1 | -1 (0.27704) | -1 | -1 |
| G: -5717.87902 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.99368 HOMO: -6.73754 LUMO: -0.61226 factor:1 | 1 (-0.74897) | -1 | -1 |
| G: -5717.87902 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.64084 HOMO: -7.37429 LUMO: 0.31293 factor:1 | -1 (0.60388) | 1 | 1 |
| G: -5717.87902 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.92346 HOMO: -6.23413 LUMO: -0.90886 factor:1 | -1 (0.32126) | -1 | -1 |
| G: -5717.87902 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.14275 HOMO: -6.51985 LUMO: -0.68028 factor:1 | -1 (0.10196) | -1 | -1 |
| G: -5717.87902 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.13206 HOMO: -6.52257 LUMO: -0.77280 factor:1 | -1 (0.11266) | -1 | -1 |
| G: -5717.87902 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.75181 HOMO: -7.29537 LUMO: 0.31837 factor:1 | -1 (0.49291) | 1 | 1 |
| G: -5717.87902 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.65670 HOMO: -6.08447 LUMO: 0.25851 factor:1 | -1 (0.58801) | -1 | -1 |
| G: -5717.87902 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.75736 HOMO: -6.20964 LUMO: 0.13606 factor:1 | -1 (0.48736) | -1 | -1 |
| G: -5717.87902 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.44228 HOMO: -6.49808 LUMO: -0.14150 factor:1 | -1 (0.80244) | -1 | -1 |
| G: -5717.87902 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.11376 HOMO: -7.10761 LUMO: 0.28028 factor:1 | -1 (1.13096) | 1 | 1 |
| G: -5717.87902 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.30892 HOMO: -6.60965 LUMO: -0.62858 factor:1 | -1 (0.93580) | -1 | -1 |
| G: -5717.87902 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.83506 HOMO: -6.40012 LUMO: -0.26939 factor:1 | -1 (1.40966) | -1 | -1 |
| G: -5717.87902 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11979.12338 HOMO: -6.65318 LUMO: -0.73199 factor:1 | -1 (3.12134) | -1 | -1 |
| G: -5717.87902 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.26732 HOMO: -6.51441 LUMO: -0.44899 factor:1 | -1 (1.97740) | -1 | -1 |
| G: -5717.87902 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.12269 HOMO: -6.28583 LUMO: -0.48708 factor:1 | -1 (2.12203) | -1 | -1 |
| G: -5717.87902 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.23892 HOMO: -6.96884 LUMO: 0.19864 factor:1 | -1 (0.00580) | -1 | -1 |
| G: -5717.87902 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.39130 HOMO: -6.89809 LUMO: 0.34558 factor:1 | 1 (-0.14659) | -1 | -1 |
| G: -5717.87902 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.96237 HOMO: -6.67495 LUMO: -0.15510 factor:1 | -1 (0.28235) | -1 | -1 |
| G: -5717.87902 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11979.05121 HOMO: -7.34980 LUMO: 0.19864 factor:1 | -1 (3.19350) | 1 | 1 |
| G: -5717.87902 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11979.96481 HOMO: -6.71305 LUMO: -0.81634 factor:1 | -1 (2.27991) | -1 | -1 |
| G: -5717.87902 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.73298 HOMO: -6.39468 LUMO: -0.47076 factor:1 | -1 (0.51174) | -1 | -1 |
| G: -5717.87902 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.29495 HOMO: -6.31304 LUMO: 1.39594 factor:1 | 1 (-0.05023) | -1 | -1 |
| G: -5717.87902 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.30617 HOMO: -6.57155 LUMO: 1.55105 factor:1 | -1 (0.93855) | -1 | -1 |
| G: -5717.87902 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.90060 HOMO: -6.68312 LUMO: 1.69255 factor:1 | -1 (0.34412) | -1 | -1 |
| G: -5717.87902 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.47683 HOMO: -6.61509 LUMO: 1.73881 factor:1 | 1 (-0.23211) | -1 | -1 |
| G: -5717.87902 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.56753 HOMO: -6.17971 LUMO: 1.90208 factor:1 | -1 (0.67718) | -1 | -1 |
| G: -5717.87902 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.16556 HOMO: -6.53073 LUMO: 1.73337 factor:1 | -1 (0.07916) | -1 | -1 |
| G: -5717.87902 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.43262 HOMO: -5.91303 LUMO: 1.90480 factor:1 | -1 (0.81210) | -1 | -1 |
| G: -5717.87902 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.09117 HOMO: -6.42733 LUMO: 1.80139 factor:1 | -1 (1.15355) | -1 | -1 |
| G: -5717.87902 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.96494 HOMO: -6.78924 LUMO: 2.31569 factor:1 | -1 (1.27978) | -1 | -1 |
| G: -5717.87902 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.67654 HOMO: -6.04093 LUMO: 1.91568 factor:1 | -1 (0.56817) | -1 | -1 |
| G: -5717.87902 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.20908 HOMO: -6.90081 LUMO: 2.36739 factor:1 | -1 (1.03564) | -1 | -1 |
| G: -5717.87902 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.22306 HOMO: -6.60965 LUMO: 2.18507 factor:1 | -1 (1.02165) | -1 | -1 |
| G: -5717.87902 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.87049 HOMO: -6.75387 LUMO: 2.48712 factor:1 | -1 (1.37423) | -1 | -1 |
| G: -5717.87902 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.05265 HOMO: -6.56883 LUMO: 1.71432 factor:1 | -1 (2.19207) | -1 | -1 |
| G: -5717.87902 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.05218 HOMO: -6.41644 LUMO: 1.72792 factor:1 | -1 (2.19253) | -1 | -1 |
| G: -5717.87902 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11979.89689 HOMO: -6.92530 LUMO: 2.54426 factor:1 | -1 (2.34783) | -1 | -1 |
| G: -5717.87902 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.04030 HOMO: -6.41644 LUMO: 2.70209 factor:1 | -1 (0.20441) | -1 | -1 |
| G: -5717.87902 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.21535 HOMO: -6.29671 LUMO: 2.14698 factor:1 | -1 (0.02936) | -1 | -1 |
| G: -5717.87902 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.90406 HOMO: -6.29127 LUMO: 1.87486 factor:1 | -1 (0.34066) | -1 | -1 |
| G: -5717.87902 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.26722 HOMO: -6.75931 LUMO: 2.78917 factor:1 | 1 (-0.02250) | -1 | -1 |
| G: -5717.87902 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.60438 HOMO: -6.40828 LUMO: 1.86942 factor:1 | -1 (0.64034) | -1 | -1 |
| G: -5717.87902 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.36135 HOMO: -6.45726 LUMO: 1.97010 factor:1 | -1 (0.88336) | -1 | -1 |
| G: -5717.87902 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.46875 HOMO: -6.43277 LUMO: 1.22723 factor:1 | 1 (-0.22403) | -1 | -1 |
| G: -5717.87902 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.43715 HOMO: -6.63414 LUMO: 1.62452 factor:1 | 1 (-0.19244) | -1 | -1 |
| G: -5717.87902 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.78737 HOMO: -6.54162 LUMO: 2.16058 factor:1 | -1 (0.45734) | -1 | -1 |
| G: -5717.87902 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.45461 HOMO: -6.40284 LUMO: 1.88575 factor:1 | -1 (0.79011) | -1 | -1 |
| G: -5717.87902 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.91004 HOMO: -6.20964 LUMO: 1.84221 factor:1 | -1 (0.33467) | -1 | -1 |
| G: -5717.87902 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.13622 HOMO: -6.58516 LUMO: 1.69799 factor:1 | -1 (0.10849) | -1 | -1 |
| G: -5717.87902 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.47477 HOMO: -6.44094 LUMO: 2.05446 factor:1 | -1 (0.76995) | -1 | -1 |
| G: -5717.87902 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.20091 HOMO: -6.61509 LUMO: 2.16058 factor:1 | -1 (1.04380) | -1 | -1 |
| G: -5717.87902 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.99151 HOMO: -6.65591 LUMO: 1.69527 factor:1 | -1 (0.25320) | -1 | -1 |
| G: -5717.87902 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.21549 HOMO: -5.55112 LUMO: 1.80411 factor:1 | -1 (0.02923) | -1 | -1 |
| G: -5717.87902 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.88778 HOMO: -6.68312 LUMO: 2.38100 factor:1 | -1 (0.35693) | -1 | -1 |
| G: -5717.87902 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.60114 HOMO: -6.51168 LUMO: 2.14698 factor:1 | -1 (0.64358) | -1 | -1 |
| G: -5717.87902 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.50423 HOMO: -6.04637 LUMO: 1.48302 factor:1 | 1 (-0.25951) | -1 | -1 |
| G: -5717.87902 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11983.13885 HOMO: -6.81645 LUMO: -0.74287 factor:1 | 1 (-0.89414) | -1 | -1 |
| G: -5717.87902 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.43484 HOMO: -6.96884 LUMO: -0.97961 factor:1 | 1 (-0.19013) | -1 | -1 |
| G: -5717.87902 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.74969 HOMO: -6.45998 LUMO: 0.09796 factor:1 | -1 (0.49503) | -1 | -1 |
| G: -5717.87902 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.09100 HOMO: -6.44638 LUMO: 0.09524 factor:1 | -1 (0.15372) | -1 | -1 |
| G: -5717.87902 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.89529 HOMO: -6.16338 LUMO: -0.54151 factor:1 | -1 (0.34942) | -1 | -1 |
| G: -5717.87902 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.90729 HOMO: -6.35930 LUMO: -0.47892 factor:1 | -1 (0.33742) | -1 | -1 |
| G: -5717.87902 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.11723 HOMO: -6.65318 LUMO: -0.00272 factor:1 | -1 (0.12749) | -1 | -1 |
| G: -5717.87902 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.82898 HOMO: -6.50080 LUMO: 0.14694 factor:1 | -1 (0.41574) | -1 | -1 |
| G: -5717.87902 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.59627 HOMO: -6.60420 LUMO: 0.94968 factor:1 | -1 (0.64845) | -1 | -1 |
| G: -5717.87902 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.96691 HOMO: -6.60148 LUMO: -0.77552 factor:1 | -1 (0.27780) | -1 | -1 |
| G: -5717.87902 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.69096 HOMO: -6.81645 LUMO: -1.05580 factor:1 | -1 (0.55375) | -1 | -1 |
| G: -5717.87902 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.43586 HOMO: -6.57971 LUMO: -0.82178 factor:1 | -1 (0.80886) | -1 | -1 |
| G: -5717.87902 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.05859 HOMO: -6.09263 LUMO: -0.45171 factor:1 | -1 (0.18613) | -1 | -1 |
| G: -5717.87902 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.33354 HOMO: -6.74298 LUMO: -0.61770 factor:1 | -1 (0.91117) | -1 | -1 |
| G: -5717.87902 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.17615 HOMO: -6.72393 LUMO: 1.21091 factor:1 | -1 (1.06856) | -1 | -1 |
| G: -5717.87902 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.20874 HOMO: -6.30488 LUMO: 1.70071 factor:1 | -1 (0.03597) | -1 | -1 |
| G: -5717.87902 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.17331 HOMO: -6.38107 LUMO: 1.55649 factor:1 | -1 (0.07140) | -1 | -1 |
| G: -5717.87902 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.06956 HOMO: -6.17154 LUMO: 1.46669 factor:1 | -1 (0.17516) | -1 | -1 |
| G: -5717.87902 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.00528 HOMO: -6.86543 LUMO: 1.98643 factor:1 | -1 (0.23943) | -1 | -1 |
| G: -5717.87902 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.08355 HOMO: -6.69944 LUMO: 1.65173 factor:1 | -1 (1.16116) | -1 | -1 |
| G: -5717.87902 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.13217 HOMO: -6.77836 LUMO: 2.16331 factor:1 | -1 (0.11255) | -1 | -1 |
| G: -5717.87902 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.29002 HOMO: -6.42189 LUMO: 2.36467 factor:1 | 1 (-0.04531) | -1 | -1 |
| G: -5717.87902 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11979.77457 HOMO: -7.00965 LUMO: 2.04358 factor:1 | -1 (2.47014) | -1 | -1 |
| G: -5717.87902 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11979.81681 HOMO: -6.36746 LUMO: 2.13881 factor:1 | -1 (2.42791) | -1 | -1 |
| G: -5717.87902 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11979.73966 HOMO: -6.37835 LUMO: 1.89935 factor:1 | -1 (2.50505) | -1 | -1 |
| G: -5717.87902 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.29337 HOMO: -7.03959 LUMO: 1.27349 factor:1 | 1 (-0.04865) | -1 | -1 |
| G: -5717.87902 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.21704 HOMO: -6.67495 LUMO: -0.89253 factor:1 | -1 (0.02767) | -1 | -1 |
| G: -5717.87902 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11983.13306 HOMO: -6.71849 LUMO: -0.97961 factor:1 | 1 (-0.88834) | -1 | -1 |
| G: -5717.87902 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11983.53301 HOMO: -6.47903 LUMO: 0.01633 factor:1 | 1 (-1.28830) | -1 | -1 |
| G: -5717.87902 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.71504 HOMO: -6.38379 LUMO: 0.01088 factor:1 | 1 (-0.47032) | -1 | -1 |
| G: -5717.87902 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.74442 HOMO: -6.49536 LUMO: -0.55239 factor:1 | 1 (-0.49971) | -1 | -1 |
| G: -5717.87902 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.05462 HOMO: -6.53345 LUMO: -0.53879 factor:1 | -1 (1.19009) | -1 | -1 |
| G: -5717.87902 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.91179 HOMO: -6.16610 LUMO: 2.15514 factor:1 | -1 (1.33292) | -1 | -1 |
| G: -5717.87902 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.89487 HOMO: -6.35114 LUMO: 1.98643 factor:1 | -1 (1.34985) | -1 | -1 |
| G: -5717.87902 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.97147 HOMO: -6.43277 LUMO: 2.16058 factor:1 | -1 (1.27325) | -1 | -1 |
| G: -5717.87902 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.69238 HOMO: -6.89809 LUMO: 2.20684 factor:1 | -1 (0.55234) | -1 | -1 |
| G: -5717.87902 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.69690 HOMO: -6.54434 LUMO: 1.93473 factor:1 | -1 (1.54781) | -1 | -1 |
| G: -5717.87902 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.45415 HOMO: -6.72938 LUMO: 2.03269 factor:1 | -1 (1.79056) | -1 | -1 |
| G: -5717.87902 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.70986 HOMO: -6.90353 LUMO: 2.19868 factor:1 | -1 (1.53486) | -1 | -1 |
| G: -5717.87902 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.60209 HOMO: -6.41372 LUMO: 2.02453 factor:1 | -1 (0.64262) | -1 | -1 |
| G: -5717.87902 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.93974 HOMO: -6.46543 LUMO: 1.90752 factor:1 | -1 (1.30498) | -1 | -1 |
| G: -5717.87902 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.04305 HOMO: -6.55522 LUMO: 2.11977 factor:1 | -1 (0.20166) | -1 | -1 |
| G: -5717.87902 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.93146 HOMO: -6.28855 LUMO: 2.02181 factor:1 | -1 (0.31326) | -1 | -1 |
| G: -5717.87902 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11983.19673 HOMO: -6.45726 LUMO: 1.52112 factor:1 | 1 (-0.95202) | -1 | -1 |
| G: -5717.87902 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11983.25159 HOMO: -6.37291 LUMO: 2.11705 factor:1 | 1 (-1.00688) | -1 | -1 |
| G: -5717.87902 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.47675 HOMO: -6.88448 LUMO: 2.24494 factor:1 | 1 (-0.23203) | -1 | -1 |
| G: -5717.87902 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11983.05600 HOMO: -6.86271 LUMO: 2.41637 factor:1 | 1 (-0.81128) | -1 | -1 |
| G: -5717.87902 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.92585 HOMO: -6.69400 LUMO: 2.34562 factor:1 | -1 (0.31886) | -1 | -1 |
| G: -5717.87902 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.15440 HOMO: -6.18243 LUMO: 2.53882 factor:1 | -1 (0.09031) | -1 | -1 |
| G: -5717.87902 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.86065 HOMO: -6.61237 LUMO: 2.54154 factor:1 | -1 (0.38406) | -1 | -1 |
| G: -5717.87902 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.82697 HOMO: -6.69672 LUMO: 2.16331 factor:1 | -1 (0.41775) | -1 | -1 |
| G: -5717.87902 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.96082 HOMO: -6.33481 LUMO: 2.34018 factor:1 | -1 (0.28390) | -1 | -1 |
| G: -5717.87902 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.71578 HOMO: -5.99739 LUMO: 2.37283 factor:1 | -1 (0.52893) | -1 | -1 |
| G: -5717.87902 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.74573 HOMO: -6.49808 LUMO: 2.47351 factor:1 | 1 (-0.50102) | -1 | -1 |
| G: -5717.87902 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.78683 HOMO: -6.22052 LUMO: 1.86398 factor:1 | -1 (0.45789) | -1 | -1 |
| G: -5717.87902 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.90819 HOMO: -6.32665 LUMO: 2.28031 factor:1 | -1 (0.33652) | -1 | -1 |
| G: -5717.87902 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.72201 HOMO: -5.98378 LUMO: 2.16331 factor:1 | -1 (0.52270) | -1 | -1 |
| G: -5717.87902 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.83921 HOMO: -6.08991 LUMO: 2.30208 factor:1 | -1 (0.40550) | -1 | -1 |
| G: -5717.87902 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.71847 HOMO: -7.07224 LUMO: 1.55105 factor:1 | -1 (0.52624) | 1 | 1 |
| G: -5717.87902 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.85605 HOMO: -6.84638 LUMO: 1.76874 factor:1 | -1 (0.38866) | -1 | -1 |
| G: -5717.87902 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.97034 HOMO: -6.68856 LUMO: 1.47758 factor:1 | -1 (0.27437) | -1 | -1 |
| G: -5717.87902 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.05476 HOMO: -6.69672 LUMO: 1.71976 factor:1 | -1 (1.18995) | -1 | -1 |
| G: -5717.87902 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.76610 HOMO: -6.86543 LUMO: 2.24766 factor:1 | -1 (1.47861) | -1 | -1 |
| G: -5717.87902 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.79592 HOMO: -7.21646 LUMO: 1.71976 factor:1 | -1 (0.44880) | 1 | 1 |
| G: -5717.87902 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.56768 HOMO: -6.94162 LUMO: 2.21773 factor:1 | -1 (1.67704) | -1 | -1 |
| G: -5717.87902 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.92736 HOMO: -6.34842 LUMO: 2.04358 factor:1 | -1 (1.31736) | -1 | -1 |
| G: -5717.87902 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.87089 HOMO: -6.53345 LUMO: 1.96738 factor:1 | -1 (1.37382) | -1 | -1 |
| G: -5717.87902 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11983.10922 HOMO: -6.34842 LUMO: 1.88303 factor:1 | 1 (-0.86451) | -1 | -1 |
| G: -5717.87902 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11983.27646 HOMO: -6.38651 LUMO: 2.08983 factor:1 | 1 (-1.03175) | -1 | -1 |
| G: -5717.87902 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.39647 HOMO: -6.01372 LUMO: 1.43676 factor:1 | 1 (-0.15176) | -1 | -1 |
| G: -5717.87902 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.88889 HOMO: -6.30216 LUMO: 1.41771 factor:1 | 1 (-0.64418) | -1 | -1 |
| G: -5717.87902 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.94335 HOMO: -6.52801 LUMO: 1.77146 factor:1 | -1 (0.30137) | -1 | -1 |
| G: -5717.87902 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.04254 HOMO: -6.53617 LUMO: 1.72792 factor:1 | -1 (1.20217) | -1 | -1 |
| G: -5717.87902 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.68166 HOMO: -6.56611 LUMO: 2.20412 factor:1 | -1 (0.56306) | -1 | -1 |
| G: -5717.87902 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.69010 HOMO: -6.66679 LUMO: -0.72927 factor:1 | -1 (1.55461) | -1 | -1 |
| G: -5717.87902 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.00921 HOMO: -6.85455 LUMO: -0.85444 factor:1 | -1 (1.23551) | -1 | -1 |
| G: -5717.87902 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.92847 HOMO: -7.21646 LUMO: 0.27211 factor:1 | -1 (1.31624) | 1 | 1 |
| G: -5717.87902 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.93187 HOMO: -6.57971 LUMO: -0.41361 factor:1 | -1 (0.31285) | -1 | -1 |
| G: -5717.87902 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.12244 HOMO: -7.03142 LUMO: -1.14288 factor:1 | -1 (1.12228) | -1 | -1 |
| G: -5717.87902 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.90783 HOMO: -6.29944 LUMO: 0.06803 factor:1 | 1 (-0.66311) | -1 | -1 |
| G: -5717.87902 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.07772 HOMO: -6.47359 LUMO: 0.28028 factor:1 | -1 (0.16700) | -1 | -1 |
| G: -5717.87902 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.67888 HOMO: -6.42189 LUMO: 1.61364 factor:1 | -1 (0.56583) | -1 | -1 |
| G: -5717.87902 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.96539 HOMO: -6.41100 LUMO: 1.80956 factor:1 | -1 (0.27932) | -1 | -1 |
| G: -5717.87902 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.92892 HOMO: -6.83278 LUMO: 1.83949 factor:1 | 1 (-0.68420) | -1 | -1 |
| G: -5717.87902 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.99045 HOMO: -6.78380 LUMO: -0.76192 factor:1 | -1 (0.25426) | -1 | -1 |
| G: -5717.87902 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.86667 HOMO: -6.95795 LUMO: 2.13609 factor:1 | -1 (0.37805) | -1 | -1 |
| G: -5717.87902 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.75545 HOMO: -6.57155 LUMO: 1.89119 factor:1 | 1 (-0.51073) | -1 | -1 |
| G: -5717.87902 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.67447 HOMO: -6.65591 LUMO: 1.93745 factor:1 | -1 (0.57024) | -1 | -1 |
| G: -5717.87902 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.01914 HOMO: -6.44638 LUMO: 2.26943 factor:1 | -1 (1.22557) | -1 | -1 |
| G: -5717.87902 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.48151 HOMO: -5.88038 LUMO: 1.90480 factor:1 | 1 (-0.23679) | -1 | -1 |
| G: -5717.87902 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.92433 HOMO: -6.22052 LUMO: 2.17691 factor:1 | -1 (0.32039) | -1 | -1 |
| G: -5717.87902 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.52992 HOMO: -6.04637 LUMO: 2.23950 factor:1 | 1 (-0.28520) | -1 | -1 |
| G: -5717.87902 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.51816 HOMO: -6.44366 LUMO: 2.24766 factor:1 | 1 (-0.27345) | -1 | -1 |
| G: -5717.87902 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.94838 HOMO: -6.81917 LUMO: 2.08439 factor:1 | -1 (0.29633) | -1 | -1 |
| G: -5717.87902 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.37618 HOMO: -6.48447 LUMO: 2.28576 factor:1 | -1 (0.86853) | -1 | -1 |
| G: -5717.87902 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.31389 HOMO: -6.54434 LUMO: 1.99187 factor:1 | 1 (-0.06917) | -1 | -1 |
| G: -5717.87902 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.23122 HOMO: -6.17698 LUMO: -0.65852 factor:1 | -1 (0.01350) | -1 | -1 |
| G: -5717.87902 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.65406 HOMO: -6.08174 LUMO: -0.58504 factor:1 | -1 (0.59065) | -1 | -1 |
| G: -5717.87902 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.13205 HOMO: -6.55250 LUMO: -0.86804 factor:1 | -1 (2.11266) | -1 | -1 |
| G: -5717.87902 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11979.20722 HOMO: -6.57699 LUMO: -0.89525 factor:1 | -1 (3.03750) | -1 | -1 |
| G: -5717.87902 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11979.22316 HOMO: -6.63141 LUMO: -1.04220 factor:1 | -1 (3.02155) | -1 | -1 |
| G: -5717.87902 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11979.29914 HOMO: -6.69128 LUMO: -0.76736 factor:1 | -1 (2.94558) | -1 | -1 |
| G: -5717.87902 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11979.67860 HOMO: -6.25318 LUMO: -1.03131 factor:1 | -1 (2.56612) | -1 | -1 |
| G: -5717.87902 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11978.94659 HOMO: -6.69944 LUMO: 0.01905 factor:1 | -1 (3.29813) | -1 | -1 |
| G: -5717.87902 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11979.02572 HOMO: -6.28583 LUMO: 0.38368 factor:1 | -1 (3.21900) | -1 | -1 |
| G: -5717.87902 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.14808 HOMO: -6.90081 LUMO: -0.83811 factor:1 | -1 (2.09664) | -1 | -1 |
| G: -5717.87902 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.21300 HOMO: -6.78380 LUMO: -0.10068 factor:1 | -1 (2.03171) | -1 | -1 |
| G: -5717.87902 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.39450 HOMO: -6.30488 LUMO: -0.98505 factor:1 | -1 (1.85021) | -1 | -1 |
| G: -5717.87902 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.26816 HOMO: -6.29671 LUMO: -1.79051 factor:1 | -1 (1.97655) | -1 | -1 |
| G: -5717.87902 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.36370 HOMO: -6.76747 LUMO: -0.22041 factor:1 | -1 (1.88101) | -1 | -1 |
| G: -5717.87902 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.04699 HOMO: -6.22597 LUMO: -0.94968 factor:1 | -1 (2.19773) | -1 | -1 |
| G: -5717.87902 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.25701 HOMO: -6.73482 LUMO: 0.05987 factor:1 | 1 (-0.01230) | -1 | -1 |
| G: -5717.87902 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.96455 HOMO: -6.28855 LUMO: 0.34831 factor:1 | -1 (0.28017) | -1 | -1 |
| G: -5717.87902 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.44635 HOMO: -6.69400 LUMO: 0.25307 factor:1 | 1 (-0.20164) | -1 | -1 |
| G: -5717.87902 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.45337 HOMO: -6.70216 LUMO: 0.61226 factor:1 | 1 (-0.20866) | -1 | -1 |
| G: -5717.87902 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.96335 HOMO: -6.70216 LUMO: 0.17415 factor:1 | -1 (0.28137) | -1 | -1 |
| G: -5717.87902 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.62026 HOMO: -6.70761 LUMO: 0.24762 factor:1 | 1 (-0.37554) | -1 | -1 |
| G: -5717.87902 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.40172 HOMO: -6.68856 LUMO: -0.84900 factor:1 | 1 (-0.15701) | -1 | -1 |
| G: -5717.87902 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.68895 HOMO: -6.71033 LUMO: -0.38640 factor:1 | -1 (0.55577) | -1 | -1 |
| G: -5717.87902 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.44227 HOMO: -6.24501 LUMO: -0.09252 factor:1 | 1 (-0.19755) | -1 | -1 |
| G: -5717.87902 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.41027 HOMO: -6.81645 LUMO: -0.07347 factor:1 | 1 (-0.16555) | -1 | -1 |
| G: -5717.87902 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.10983 HOMO: -6.49536 LUMO: 0.09796 factor:1 | -1 (0.13489) | -1 | -1 |
| G: -5717.87902 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.79145 HOMO: -6.71033 LUMO: -0.26395 factor:1 | -1 (0.45326) | -1 | -1 |
| G: -5717.87902 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.94561 HOMO: -6.70489 LUMO: -0.09252 factor:1 | -1 (0.29911) | -1 | -1 |
| G: -5717.87902 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.08836 HOMO: -6.23685 LUMO: 0.39729 factor:1 | -1 (0.15636) | -1 | -1 |
| G: -5717.87902 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.76688 HOMO: -6.69400 LUMO: -0.05442 factor:1 | -1 (0.47783) | -1 | -1 |
| G: -5717.87902 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.35760 HOMO: -6.36202 LUMO: 0.09796 factor:1 | -1 (0.88712) | -1 | -1 |
| G: -5717.87902 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.22936 HOMO: -6.54978 LUMO: 0.15510 factor:1 | -1 (2.01536) | -1 | -1 |
| G: -5717.87902 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.55785 HOMO: -6.77836 LUMO: 0.25851 factor:1 | -1 (0.68687) | -1 | -1 |
| G: -5717.87902 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.93061 HOMO: -5.70623 LUMO: 0.73471 factor:1 | -1 (0.31410) | -1 | -1 |
| G: -5717.87902 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11979.94832 HOMO: -5.58378 LUMO: 0.89253 factor:1 | -1 (2.29640) | -1 | -1 |
| G: -5717.87902 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.42597 HOMO: -5.68718 LUMO: 0.87893 factor:1 | 1 (-0.18126) | -1 | -1 |
| G: -5717.87902 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.53879 HOMO: -5.10486 LUMO: 1.11567 factor:1 | 1 (-0.29407) | -1 | -1 |
| G: -5717.87902 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.36958 HOMO: -4.59328 LUMO: 1.27621 factor:1 | -1 (1.87514) | -1 | -1 |
| G: -5717.87902 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.49454 HOMO: -4.45450 LUMO: 1.82044 factor:1 | 1 (-0.24983) | -1 | -1 |
| G: -5717.87902 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.34736 HOMO: -4.64226 LUMO: 1.70615 factor:1 | 1 (-0.10264) | -1 | -1 |
| G: -5717.87902 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.15065 HOMO: -5.04227 LUMO: 1.04492 factor:1 | -1 (0.09407) | -1 | -1 |
| G: -5717.87902 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.22073 HOMO: -4.85723 LUMO: 0.93607 factor:1 | -1 (2.02398) | -1 | -1 |
| G: -5717.87902 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.33573 HOMO: -4.72934 LUMO: 1.00410 factor:1 | -1 (1.90899) | -1 | -1 |
| G: -5717.87902 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.13665 HOMO: -4.56335 LUMO: 1.56738 factor:1 | -1 (2.10807) | -1 | -1 |
| G: -5717.87902 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.01801 HOMO: -5.48854 LUMO: 0.33198 factor:1 | -1 (2.22671) | -1 | -1 |
| G: -5717.87902 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.92909 HOMO: -4.97424 LUMO: 1.33608 factor:1 | -1 (0.31562) | -1 | -1 |
| G: -5717.87902 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.06143 HOMO: -4.60145 LUMO: 1.74697 factor:1 | -1 (1.18329) | -1 | -1 |
| G: -5717.87902 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.93228 HOMO: -5.60010 LUMO: 0.74831 factor:1 | -1 (1.31243) | -1 | -1 |
| G: -5717.87902 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.25068 HOMO: -5.66541 LUMO: 0.66668 factor:1 | -1 (0.99403) | -1 | -1 |
| G: -5717.87902 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.99094 HOMO: -6.50080 LUMO: 0.07075 factor:1 | -1 (0.25377) | -1 | -1 |
| G: -5717.87902 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.17261 HOMO: -5.79603 LUMO: 0.22313 factor:1 | -1 (1.07210) | -1 | -1 |
| G: -5717.87902 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.80479 HOMO: -4.68036 LUMO: 1.29798 factor:1 | -1 (0.43993) | -1 | -1 |
| G: -5717.87902 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.82989 HOMO: -4.84363 LUMO: 1.34424 factor:1 | -1 (1.41483) | -1 | -1 |
| G: -5717.87902 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.44784 HOMO: -4.62321 LUMO: 1.82861 factor:1 | -1 (1.79688) | -1 | -1 |
| G: -5717.87902 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.41959 HOMO: -5.83684 LUMO: 0.82178 factor:1 | -1 (1.82512) | -1 | -1 |
| G: -5717.87902 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.00805 HOMO: -5.27629 LUMO: 0.57960 factor:1 | -1 (2.23667) | -1 | -1 |
| G: -5717.87902 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11979.93354 HOMO: -5.15928 LUMO: -2.96876 factor:1 | -1 (2.31117) | -1 | -1 |
| G: -5717.87902 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.35034 HOMO: -5.08853 LUMO: 0.89253 factor:1 | -1 (1.89438) | -1 | -1 |
| G: -5717.87902 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.28030 HOMO: -6.42461 LUMO: 0.04354 factor:1 | -1 (1.96442) | -1 | -1 |
| G: -5717.87902 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.89065 HOMO: -6.42733 LUMO: -0.00544 factor:1 | -1 (1.35407) | -1 | -1 |
| G: -5717.87902 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.15414 HOMO: -5.87494 LUMO: 0.69933 factor:1 | -1 (1.09058) | -1 | -1 |
| G: -5717.87902 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.17630 HOMO: -5.07492 LUMO: 1.02587 factor:1 | -1 (2.06842) | -1 | -1 |
| G: -5717.87902 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.30713 HOMO: -4.44362 LUMO: 1.99187 factor:1 | -1 (1.93759) | -1 | -1 |
| G: -5717.87902 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.09602 HOMO: -5.82052 LUMO: 0.43810 factor:1 | -1 (2.14869) | -1 | -1 |
| G: -5717.87902 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.59963 HOMO: -5.75793 LUMO: 0.76464 factor:1 | 1 (-0.35492) | -1 | -1 |
| G: -5717.87902 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.55958 HOMO: -5.09669 LUMO: 0.72382 factor:1 | 1 (-0.31486) | -1 | -1 |
| G: -5717.87902 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.26534 HOMO: -6.75387 LUMO: -2.02453 factor:1 | 1 (-0.02063) | -1 | -1 |
| G: -5717.87902 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.26042 HOMO: -5.02322 LUMO: 1.14832 factor:1 | 1 (-0.01570) | -1 | -1 |
| G: -5717.87902 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.53433 HOMO: -5.75521 LUMO: 0.73471 factor:1 | 1 (-0.28961) | -1 | -1 |
| G: -5717.87902 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11983.12108 HOMO: -5.89943 LUMO: 0.54967 factor:1 | 1 (-0.87637) | -1 | -1 |
| G: -5717.87902 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11983.01480 HOMO: -5.80147 LUMO: 0.72382 factor:1 | 1 (-0.77008) | -1 | -1 |
| G: -5717.87902 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.30327 HOMO: -6.16066 LUMO: 0.39457 factor:1 | 1 (-0.05856) | -1 | -1 |
| G: -5717.87902 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11983.58071 HOMO: -5.98650 LUMO: 0.76736 factor:1 | 1 (-1.33600) | -1 | -1 |
| G: -5717.87902 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.71520 HOMO: -4.74839 LUMO: 1.88847 factor:1 | 1 (-0.47048) | -1 | -1 |
| G: -5717.87902 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11983.45557 HOMO: -5.62459 LUMO: 0.26939 factor:1 | 1 (-1.21085) | -1 | -1 |
| G: -5717.87902 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.62595 HOMO: -4.88172 LUMO: 1.30070 factor:1 | 1 (-0.38123) | -1 | -1 |
| G: -5717.87902 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11983.12089 HOMO: -5.09397 LUMO: 0.98505 factor:1 | 1 (-0.87618) | -1 | -1 |
| G: -5717.87902 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.37762 HOMO: -6.50080 LUMO: -0.28300 factor:1 | 1 (-0.13290) | -1 | -1 |
| G: -5717.87902 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.55541 HOMO: -5.04227 LUMO: 1.49935 factor:1 | 1 (-0.31070) | -1 | -1 |
| G: -5717.87902 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.80328 HOMO: -5.22731 LUMO: 0.88437 factor:1 | 1 (-0.55857) | -1 | -1 |
| G: -5717.87902 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.07941 HOMO: -4.95519 LUMO: 1.25717 factor:1 | -1 (0.16531) | -1 | -1 |
| G: -5717.87902 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.53141 HOMO: -4.61233 LUMO: 1.27621 factor:1 | 1 (-0.28670) | -1 | -1 |
| G: -5717.87902 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.31140 HOMO: -4.70757 LUMO: 1.63813 factor:1 | -1 (1.93331) | -1 | -1 |
| G: -5717.87902 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.45377 HOMO: -4.85179 LUMO: 1.11839 factor:1 | -1 (1.79094) | -1 | -1 |
| G: -5717.87902 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.64411 HOMO: -4.97696 LUMO: 1.00138 factor:1 | -1 (0.60061) | -1 | -1 |
| G: -5717.87902 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.61651 HOMO: -5.64636 LUMO: 0.81090 factor:1 | -1 (0.62820) | -1 | -1 |
| G: -5717.87902 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.30619 HOMO: -4.37831 LUMO: 1.90208 factor:1 | -1 (0.93852) | -1 | -1 |
| G: -5717.87902 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.02047 HOMO: -4.67764 LUMO: 1.54561 factor:1 | -1 (0.22425) | -1 | -1 |
| G: -5717.87902 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.31468 HOMO: -5.87766 LUMO: 0.42994 factor:1 | -1 (0.93003) | -1 | -1 |
| G: -5717.87902 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.92964 HOMO: -6.03821 LUMO: 0.32382 factor:1 | -1 (1.31507) | -1 | -1 |
| G: -5717.87902 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.02213 HOMO: -5.99739 LUMO: 0.69389 factor:1 | -1 (1.22258) | -1 | -1 |
| G: -5717.87902 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.86915 HOMO: -6.43821 LUMO: 0.15238 factor:1 | -1 (1.37556) | -1 | -1 |
| G: -5717.87902 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.16127 HOMO: -6.63414 LUMO: -0.07347 factor:1 | -1 (1.08345) | -1 | -1 |
| G: -5717.87902 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.95778 HOMO: -6.50080 LUMO: 0.10068 factor:1 | -1 (1.28694) | -1 | -1 |
| G: -5717.87902 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.16768 HOMO: -6.49264 LUMO: 0.19592 factor:1 | -1 (0.07704) | -1 | -1 |
| G: -5717.87902 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.91094 HOMO: -5.83956 LUMO: 0.12517 factor:1 | -1 (0.33377) | -1 | -1 |
| G: -5717.87902 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.11829 HOMO: -6.50896 LUMO: 0.19048 factor:1 | -1 (0.12642) | -1 | -1 |
| G: -5717.87902 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.18912 HOMO: -6.56611 LUMO: 0.04898 factor:1 | -1 (0.05559) | -1 | -1 |
| G: -5717.87902 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.73189 HOMO: -6.68040 LUMO: -0.08436 factor:1 | -1 (0.51283) | -1 | -1 |
| G: -5717.87902 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11983.15613 HOMO: -6.73754 LUMO: -0.08708 factor:1 | 1 (-0.91142) | -1 | -1 |
| G: -5717.87902 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.45525 HOMO: -6.80285 LUMO: -0.10612 factor:1 | 1 (-0.21053) | -1 | -1 |
| G: -5717.87902 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.41585 HOMO: -6.35658 LUMO: 0.02177 factor:1 | 1 (-0.17113) | -1 | -1 |
| G: -5717.87902 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11983.19412 HOMO: -5.74160 LUMO: 0.14694 factor:1 | 1 (-0.94941) | -1 | -1 |
| G: -5717.87902 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.47027 HOMO: -4.78376 LUMO: 0.92791 factor:1 | 1 (-0.22556) | -1 | -1 |
| G: -5717.87902 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.17519 HOMO: -5.90215 LUMO: 0.36463 factor:1 | -1 (0.06953) | -1 | -1 |
| G: -5717.87902 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.70619 HOMO: -4.99329 LUMO: 0.85988 factor:1 | 1 (-0.46148) | -1 | -1 |
| G: -5717.87902 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.82285 HOMO: -4.93887 LUMO: 1.33608 factor:1 | 1 (-0.57813) | -1 | -1 |
| G: -5717.87902 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.11225 HOMO: -5.19193 LUMO: 0.50341 factor:1 | -1 (0.13247) | -1 | -1 |
| G: -5717.87902 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.79945 HOMO: -6.64502 LUMO: -1.98643 factor:1 | -1 (0.44526) | -1 | -1 |
| G: -5717.87902 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.13816 HOMO: -5.15384 LUMO: 0.94968 factor:1 | -1 (0.10656) | -1 | -1 |
| G: -5717.87902 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.02812 HOMO: -6.31032 LUMO: 0.08436 factor:1 | -1 (1.21659) | -1 | -1 |
| G: -5717.87902 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.44533 HOMO: -4.88716 LUMO: 0.82995 factor:1 | -1 (0.79939) | -1 | -1 |
| G: -5717.87902 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.50927 HOMO: -5.57017 LUMO: 0.19320 factor:1 | -1 (0.73544) | -1 | -1 |
| G: -5717.87902 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.20286 HOMO: -4.92254 LUMO: 0.93879 factor:1 | -1 (0.04185) | -1 | -1 |
| G: -5717.87902 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.40782 HOMO: -4.77288 LUMO: 1.60003 factor:1 | 1 (-0.16311) | -1 | -1 |
| G: -5717.87902 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.30080 HOMO: -4.97696 LUMO: 0.89798 factor:1 | 1 (-0.05608) | -1 | -1 |
| G: -5717.87902 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.77199 HOMO: -5.00690 LUMO: 1.14288 factor:1 | 1 (-0.52728) | -1 | -1 |
| G: -5717.87902 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.19892 HOMO: -4.88444 LUMO: 1.48574 factor:1 | -1 (0.04580) | -1 | -1 |
| G: -5717.87902 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.08455 HOMO: -5.03955 LUMO: 1.51023 factor:1 | -1 (0.16017) | -1 | -1 |
| G: -5717.87902 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.32725 HOMO: -5.22459 LUMO: 0.99049 factor:1 | 1 (-0.08253) | -1 | -1 |
| G: -5717.87902 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.30599 HOMO: -5.29534 LUMO: 0.96056 factor:1 | 1 (-0.06128) | -1 | -1 |
| G: -5717.87902 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.08654 HOMO: -5.35520 LUMO: 0.68301 factor:1 | -1 (1.15817) | -1 | -1 |
| G: -5717.87902 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.75114 HOMO: -5.27357 LUMO: 1.18642 factor:1 | -1 (1.49358) | -1 | -1 |
| G: -5717.87902 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11978.91380 HOMO: -5.79875 LUMO: 0.61770 factor:1 | -1 (3.33092) | -1 | -1 |
| G: -5717.87902 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11978.73709 HOMO: -7.64640 LUMO: -2.45175 factor:1 | -1 (3.50763) | -1 | -1 |
| G: -5717.87902 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.05096 HOMO: -7.46953 LUMO: -1.29798 factor:1 | -1 (2.19375) | 1 | 1 |
| G: -5717.87902 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.89426 HOMO: -7.95389 LUMO: -0.37280 factor:1 | -1 (0.35046) | 1 | 1 |
| G: -5717.87902 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.39743 HOMO: -7.23279 LUMO: -1.19186 factor:1 | 1 (-0.15271) | 1 | 1 |
| G: -5717.87902 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.52810 HOMO: -7.14299 LUMO: -1.12927 factor:1 | -1 (0.71661) | 1 | 1 |
| G: -5717.87902 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.14510 HOMO: -6.93074 LUMO: 0.31565 factor:1 | -1 (1.09961) | -1 | -1 |
| G: -5717.87902 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11979.83773 HOMO: -6.63141 LUMO: 0.28028 factor:1 | -1 (2.40698) | -1 | -1 |
| G: -5717.87902 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11979.84938 HOMO: -7.10489 LUMO: -1.07213 factor:1 | -1 (2.39534) | 1 | 1 |
| G: -5717.87902 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.00029 HOMO: -7.00693 LUMO: -0.69389 factor:1 | -1 (2.24442) | -1 | -1 |
| G: -5717.87902 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.03232 HOMO: -8.50356 LUMO: -1.79595 factor:1 | -1 (2.21239) | -1 | -1 |
| G: -5717.87902 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11979.93365 HOMO: -7.79334 LUMO: -2.33746 factor:1 | -1 (2.31106) | -1 | -1 |
| G: -5717.87902 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.17992 HOMO: -7.24367 LUMO: -0.85172 factor:1 | -1 (0.06479) | 1 | 1 |
| G: -5717.87902 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.17473 HOMO: -7.94028 LUMO: -0.20136 factor:1 | -1 (0.06999) | 1 | 1 |
| G: -5717.87902 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.07105 HOMO: -7.22462 LUMO: 0.84627 factor:1 | -1 (0.17366) | 1 | 1 |
| G: -5717.87902 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.34657 HOMO: -6.54978 LUMO: 0.34831 factor:1 | 1 (-0.10185) | -1 | -1 |
| G: -5717.87902 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.68304 HOMO: -6.86815 LUMO: 0.32109 factor:1 | -1 (0.56167) | -1 | -1 |
| G: -5717.87902 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.50203 HOMO: -7.17564 LUMO: -1.28438 factor:1 | -1 (0.74268) | 1 | 1 |
| G: -5717.87902 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.42935 HOMO: -7.03142 LUMO: -1.12655 factor:1 | -1 (0.81536) | -1 | -1 |
| G: -5717.87902 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.15614 HOMO: -7.39878 LUMO: 0.15783 factor:1 | -1 (0.08857) | 1 | 1 |
| G: -5717.87902 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.12093 HOMO: -7.25728 LUMO: 0.42178 factor:1 | -1 (0.12378) | 1 | 1 |
| G: -5717.87902 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.42421 HOMO: -6.86543 LUMO: 0.93879 factor:1 | -1 (0.82050) | -1 | -1 |
| G: -5717.87902 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.00964 HOMO: -7.09673 LUMO: -0.69661 factor:1 | -1 (1.23507) | 1 | 1 |
| G: -5717.87902 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.23052 HOMO: -7.74708 LUMO: 0.01088 factor:1 | -1 (1.01420) | 1 | 1 |
| G: -5717.87902 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.74264 HOMO: -6.80557 LUMO: 0.46531 factor:1 | -1 (0.50208) | -1 | -1 |
| G: -5717.87902 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.28520 HOMO: -7.29265 LUMO: 1.31975 factor:1 | -1 (1.95952) | 1 | 1 |
| G: -5717.87902 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.26057 HOMO: -6.93618 LUMO: 0.29388 factor:1 | -1 (1.98415) | -1 | -1 |
| G: -5717.87902 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.28566 HOMO: -6.53073 LUMO: 0.71022 factor:1 | -1 (1.95906) | -1 | -1 |
| G: -5717.87902 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.26922 HOMO: -6.41917 LUMO: -1.24084 factor:1 | -1 (1.97549) | -1 | -1 |
| G: -5717.87902 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.24781 HOMO: -6.67495 LUMO: -1.09118 factor:1 | -1 (1.99691) | -1 | -1 |
| G: -5717.87902 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11979.94788 HOMO: -6.97156 LUMO: -0.53606 factor:1 | -1 (2.29683) | -1 | -1 |
| G: -5717.87902 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.23747 HOMO: -6.85183 LUMO: -0.45715 factor:1 | -1 (2.00725) | -1 | -1 |
| G: -5717.87902 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.14846 HOMO: -7.12666 LUMO: -0.67484 factor:1 | -1 (2.09626) | 1 | 1 |
| G: -5717.87902 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.01651 HOMO: -7.49946 LUMO: -0.14694 factor:1 | -1 (2.22820) | 1 | 1 |
| G: -5717.87902 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.51710 HOMO: -7.44231 LUMO: 0.58232 factor:1 | 1 (-0.27239) | 1 | 1 |
| G: -5717.87902 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.37163 HOMO: -7.36340 LUMO: -0.68301 factor:1 | 1 (-0.12691) | 1 | 1 |
| G: -5717.87902 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.70106 HOMO: -6.13073 LUMO: -0.54967 factor:1 | -1 (0.54366) | -1 | -1 |
| G: -5717.87902 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.33434 HOMO: -7.81511 LUMO: -0.06531 factor:1 | -1 (1.91038) | 1 | 1 |
| G: -5717.87902 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.34398 HOMO: -7.26816 LUMO: -1.02587 factor:1 | 1 (-0.09927) | 1 | 1 |
| G: -5717.87902 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.59133 HOMO: -7.98110 LUMO: -0.17960 factor:1 | 1 (-0.34662) | 1 | 1 |
| G: -5717.87902 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.32568 HOMO: -7.44776 LUMO: -1.00954 factor:1 | -1 (0.91904) | 1 | 1 |
| G: -5717.87902 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.33745 HOMO: -7.47769 LUMO: -1.02859 factor:1 | 1 (-0.09274) | 1 | 1 |
| G: -5717.87902 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.23620 HOMO: -6.75659 LUMO: 0.39457 factor:1 | -1 (0.00852) | -1 | -1 |
| G: -5717.87902 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.22873 HOMO: -6.71849 LUMO: 0.36735 factor:1 | -1 (2.01598) | -1 | -1 |
| G: -5717.87902 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.32424 HOMO: -7.64096 LUMO: -1.43948 factor:1 | -1 (1.92047) | 1 | 1 |
| G: -5717.87902 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11979.77817 HOMO: -7.83144 LUMO: -1.36601 factor:1 | -1 (2.46655) | 1 | 1 |
| G: -5717.87902 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11979.77632 HOMO: -7.19469 LUMO: 0.35103 factor:1 | -1 (2.46840) | 1 | 1 |
| G: -5717.87902 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.10870 HOMO: -7.03414 LUMO: 0.20409 factor:1 | -1 (2.13601) | -1 | -1 |
| G: -5717.87902 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11979.84336 HOMO: -7.22734 LUMO: 0.31293 factor:1 | -1 (2.40135) | 1 | 1 |
| G: -5717.87902 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.03218 HOMO: -6.93618 LUMO: 0.56055 factor:1 | -1 (2.21253) | -1 | -1 |
| G: -5717.87902 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11979.98078 HOMO: -6.94707 LUMO: -0.88709 factor:1 | -1 (2.26393) | -1 | -1 |
| G: -5717.87902 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.04082 HOMO: -6.86543 LUMO: -0.83267 factor:1 | -1 (0.20389) | -1 | -1 |
| G: -5717.87902 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.10325 HOMO: -6.82189 LUMO: -1.15376 factor:1 | -1 (1.14146) | -1 | -1 |
| G: -5717.87902 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.12695 HOMO: -6.65046 LUMO: -0.46531 factor:1 | -1 (1.11776) | -1 | -1 |
| G: -5717.87902 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.01614 HOMO: -6.52529 LUMO: 0.20953 factor:1 | -1 (0.22858) | -1 | -1 |
| G: -5717.87902 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.13985 HOMO: -6.80557 LUMO: 0.44355 factor:1 | -1 (1.10486) | -1 | -1 |
| G: -5717.87902 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.83495 HOMO: -6.93074 LUMO: -0.81634 factor:1 | -1 (1.40977) | -1 | -1 |
| G: -5717.87902 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.79589 HOMO: -7.43143 LUMO: -0.45987 factor:1 | -1 (0.44882) | 1 | 1 |
| G: -5717.87902 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.01647 HOMO: -7.07224 LUMO: -0.68028 factor:1 | -1 (1.22824) | 1 | 1 |
| G: -5717.87902 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.99682 HOMO: -6.68040 LUMO: -0.71566 factor:1 | -1 (0.24790) | -1 | -1 |
| G: -5717.87902 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.23686 HOMO: -6.26406 LUMO: -1.09934 factor:1 | -1 (1.00786) | -1 | -1 |
| G: -5717.87902 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.99005 HOMO: -5.94569 LUMO: -0.72110 factor:1 | -1 (1.25466) | -1 | -1 |
| G: -5717.87902 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.37114 HOMO: -6.12256 LUMO: -0.42178 factor:1 | 1 (-0.12642) | -1 | -1 |
| G: -5717.87902 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.49120 HOMO: -6.09807 LUMO: 0.11429 factor:1 | 1 (-0.24648) | -1 | -1 |
| G: -5717.87902 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.19742 HOMO: -7.35252 LUMO: -0.55783 factor:1 | -1 (0.04729) | 1 | 1 |
| G: -5717.87902 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.13241 HOMO: -7.57837 LUMO: -0.76736 factor:1 | -1 (0.11230) | 1 | 1 |
| G: -5717.87902 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.24104 HOMO: -6.16066 LUMO: 0.01905 factor:1 | -1 (0.00367) | -1 | -1 |
| G: -5717.87902 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.11433 HOMO: -6.13345 LUMO: -0.41906 factor:1 | -1 (1.13039) | -1 | -1 |
| G: -5717.87902 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.99100 HOMO: -6.10351 LUMO: -0.33742 factor:1 | -1 (0.25372) | -1 | -1 |
| G: -5717.87902 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.31710 HOMO: -7.24639 LUMO: -0.51702 factor:1 | 1 (-0.07238) | 1 | 1 |
| G: -5717.87902 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.41432 HOMO: -6.98244 LUMO: -1.82044 factor:1 | 1 (-0.16961) | -1 | -1 |
| G: -5717.87902 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11979.78170 HOMO: -6.37563 LUMO: -1.67622 factor:1 | -1 (2.46301) | -1 | -1 |
| G: -5717.87902 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.29287 HOMO: -5.79058 LUMO: -2.55243 factor:1 | -1 (1.95185) | -1 | -1 |
| G: -5717.87902 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11979.88127 HOMO: -6.34025 LUMO: -0.27483 factor:1 | -1 (2.36344) | -1 | -1 |
| G: -5717.87902 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11979.61446 HOMO: -6.05453 LUMO: -0.51157 factor:1 | -1 (2.63025) | -1 | -1 |
| G: -5717.87902 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.21808 HOMO: -7.53755 LUMO: -0.38912 factor:1 | -1 (1.02663) | 1 | 1 |
| G: -5717.87902 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.96970 HOMO: -7.00421 LUMO: -0.50885 factor:1 | -1 (1.27502) | -1 | -1 |
| G: -5717.87902 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.05628 HOMO: -7.52123 LUMO: -0.37552 factor:1 | -1 (1.18843) | 1 | 1 |
| G: -5717.87902 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.05032 HOMO: -6.70489 LUMO: -1.04764 factor:1 | -1 (0.19440) | -1 | -1 |
| G: -5717.87902 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.12039 HOMO: -7.06408 LUMO: -1.16737 factor:1 | -1 (1.12432) | 1 | 1 |
| G: -5717.87902 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.67894 HOMO: -6.71849 LUMO: -1.02315 factor:1 | -1 (0.56578) | -1 | -1 |
| G: -5717.87902 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.76166 HOMO: -6.16610 LUMO: -0.50885 factor:1 | -1 (0.48306) | -1 | -1 |
| G: -5717.87902 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.78452 HOMO: -6.48447 LUMO: 0.07619 factor:1 | -1 (1.46019) | -1 | -1 |
| G: -5717.87902 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.03495 HOMO: -7.06135 LUMO: 0.09796 factor:1 | -1 (1.20976) | 1 | 1 |
| G: -5717.87902 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.96207 HOMO: -6.47359 LUMO: 0.22585 factor:1 | -1 (0.28264) | -1 | -1 |
| G: -5717.87902 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.10377 HOMO: -6.10896 LUMO: -0.62314 factor:1 | -1 (1.14095) | -1 | -1 |
| G: -5717.87902 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.22987 HOMO: -6.88176 LUMO: -0.96600 factor:1 | -1 (2.01484) | -1 | -1 |
| G: -5717.87902 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.08002 HOMO: -6.67495 LUMO: 0.21769 factor:1 | -1 (2.16469) | -1 | -1 |
| G: -5717.87902 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.05469 HOMO: -6.84911 LUMO: 0.38368 factor:1 | -1 (2.19003) | -1 | -1 |
| G: -5717.87902 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11979.90470 HOMO: -6.83550 LUMO: 1.29798 factor:1 | -1 (2.34002) | -1 | -1 |
| G: -5717.87902 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11979.64758 HOMO: -6.67495 LUMO: 1.46941 factor:1 | -1 (2.59714) | -1 | -1 |
| G: -5717.87902 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.27477 HOMO: -6.81917 LUMO: 1.30887 factor:1 | -1 (1.96994) | -1 | -1 |
| G: -5717.87902 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.37701 HOMO: -6.56611 LUMO: 0.66396 factor:1 | -1 (1.86771) | -1 | -1 |
| G: -5717.87902 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11979.86753 HOMO: -6.76203 LUMO: 0.60137 factor:1 | -1 (2.37719) | -1 | -1 |
| G: -5717.87902 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11979.14975 HOMO: -6.55794 LUMO: 0.34286 factor:1 | -1 (3.09497) | -1 | -1 |
| G: -5717.87902 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.48871 HOMO: -6.83550 LUMO: 0.35919 factor:1 | -1 (1.75601) | -1 | -1 |
| G: -5717.87902 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.36201 HOMO: -7.17836 LUMO: 0.63130 factor:1 | -1 (1.88270) | 1 | 1 |
| G: -5717.87902 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11979.98973 HOMO: -6.29944 LUMO: -0.69389 factor:1 | -1 (2.25498) | -1 | -1 |
| G: -5717.87902 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.93664 HOMO: -7.06680 LUMO: -0.95784 factor:1 | -1 (1.30808) | 1 | 1 |
| G: -5717.87902 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.15039 HOMO: -6.84638 LUMO: -0.87076 factor:1 | -1 (2.09432) | -1 | -1 |
| G: -5717.87902 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.32381 HOMO: -6.96339 LUMO: -1.05308 factor:1 | -1 (1.92091) | -1 | -1 |
| G: -5717.87902 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.22547 HOMO: -6.75387 LUMO: -1.04220 factor:1 | -1 (2.01925) | -1 | -1 |
| G: -5717.87902 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.34517 HOMO: -6.71849 LUMO: -0.84355 factor:1 | -1 (1.89955) | -1 | -1 |
| G: -5717.87902 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.37837 HOMO: -7.16748 LUMO: 0.51702 factor:1 | -1 (1.86635) | 1 | 1 |
| G: -5717.87902 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.52743 HOMO: -6.92530 LUMO: 0.71566 factor:1 | -1 (1.71728) | -1 | -1 |
| G: -5717.87902 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.97149 HOMO: -7.11034 LUMO: 0.01905 factor:1 | -1 (1.27322) | 1 | -1 |
| G: -5717.87902 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.15378 HOMO: -6.79468 LUMO: 0.77008 factor:1 | -1 (1.09093) | -1 | -1 |
| G: -5717.87902 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.84610 HOMO: -6.52801 LUMO: 0.98233 factor:1 | -1 (1.39861) | -1 | -1 |
| G: -5717.87902 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.25457 HOMO: -6.76475 LUMO: 0.53334 factor:1 | -1 (0.99014) | -1 | -1 |
| G: -5717.87902 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.95887 HOMO: -5.29261 LUMO: 0.57416 factor:1 | -1 (1.28585) | -1 | -1 |
| G: -5717.87902 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.30310 HOMO: -6.57971 LUMO: 0.12789 factor:1 | -1 (1.94161) | -1 | -1 |
| G: -5717.87902 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.27790 HOMO: -6.99333 LUMO: 0.51430 factor:1 | -1 (1.96681) | -1 | -1 |
| G: -5717.87902 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.97364 HOMO: -6.41917 LUMO: 0.19048 factor:1 | -1 (1.27107) | -1 | -1 |
| G: -5717.87902 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.92904 HOMO: -6.16066 LUMO: 1.77146 factor:1 | -1 (1.31567) | -1 | -1 |
| G: -5717.87902 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.25898 HOMO: -6.90353 LUMO: 1.65717 factor:1 | -1 (0.98573) | -1 | -1 |
| G: -5717.87902 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.91391 HOMO: -5.94569 LUMO: 1.29526 factor:1 | -1 (1.33080) | -1 | -1 |
| G: -5717.87902 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.63083 HOMO: -6.60420 LUMO: 1.33880 factor:1 | -1 (1.61388) | -1 | -1 |
| G: -5717.87902 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.00820 HOMO: -6.23957 LUMO: 0.09524 factor:1 | -1 (1.23651) | -1 | -1 |
| G: -5717.87902 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.40691 HOMO: -6.80013 LUMO: 1.34696 factor:1 | -1 (1.83780) | -1 | -1 |
| G: -5717.87902 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.32838 HOMO: -7.53483 LUMO: -1.52384 factor:1 | -1 (1.91633) | -1 | -1 |
| G: -5717.87902 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.20593 HOMO: -7.62463 LUMO: -1.65717 factor:1 | -1 (2.03879) | -1 | -1 |
| G: -5717.87902 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.35733 HOMO: -7.62463 LUMO: -1.61364 factor:1 | -1 (1.88738) | -1 | -1 |
| G: -5717.87902 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.05678 HOMO: -8.04096 LUMO: -1.66806 factor:1 | -1 (2.18793) | -1 | -1 |
| G: -5717.87902 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.31091 HOMO: -7.18381 LUMO: -1.17553 factor:1 | -1 (1.93380) | 1 | 1 |
| G: -5717.87902 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.24103 HOMO: -7.69538 LUMO: -1.36601 factor:1 | -1 (2.00368) | 1 | 1 |
| G: -5717.87902 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11979.87025 HOMO: -7.95117 LUMO: -1.48302 factor:1 | -1 (2.37447) | -1 | -1 |
| G: -5717.87902 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.12326 HOMO: -6.98516 LUMO: 0.35919 factor:1 | -1 (2.12145) | -1 | -1 |
| G: -5717.87902 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.70961 HOMO: -7.91579 LUMO: -0.32109 factor:1 | -1 (1.53510) | 1 | 1 |
| G: -5717.87902 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.45182 HOMO: -6.75659 LUMO: -0.03537 factor:1 | 1 (-0.20711) | -1 | -1 |
| G: -5717.87902 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.44951 HOMO: -7.78518 LUMO: -2.36467 factor:1 | 1 (-0.20479) | -1 | -1 |
| G: -5717.87902 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.36298 HOMO: -7.96477 LUMO: -2.75651 factor:1 | 1 (-0.11826) | -1 | -1 |
| G: -5717.87902 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.56140 HOMO: -7.60286 LUMO: -2.35106 factor:1 | 1 (-0.31669) | -1 | -1 |
| G: -5717.87902 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.31182 HOMO: -7.38245 LUMO: -1.21635 factor:1 | 1 (-0.06710) | 1 | 1 |
| G: -5717.87902 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.24934 HOMO: -7.91579 LUMO: -1.50479 factor:1 | 1 (-0.00463) | -1 | -1 |
| G: -5717.87902 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.43468 HOMO: -8.07362 LUMO: -0.28028 factor:1 | 1 (-0.18996) | 1 | 1 |
| G: -5717.87902 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.01731 HOMO: -7.38245 LUMO: -1.15921 factor:1 | -1 (0.22741) | 1 | 1 |
| G: -5717.87902 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.02351 HOMO: -7.18653 LUMO: -0.94968 factor:1 | -1 (0.22120) | 1 | 1 |
| G: -5717.87902 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.48692 HOMO: -6.88448 LUMO: 0.38096 factor:1 | 1 (-0.24221) | -1 | -1 |
| G: -5717.87902 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.99589 HOMO: -6.97972 LUMO: 0.43266 factor:1 | -1 (0.24882) | -1 | -1 |
| G: -5717.87902 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.45705 HOMO: -6.88992 LUMO: -0.43538 factor:1 | 1 (-0.21233) | -1 | -1 |
| G: -5717.87902 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.71385 HOMO: -7.97021 LUMO: -0.17143 factor:1 | -1 (0.53087) | 1 | 1 |
| G: -5717.87902 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.22229 HOMO: -6.92530 LUMO: 0.77280 factor:1 | -1 (0.02242) | -1 | -1 |
| G: -5717.87902 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.32809 HOMO: -7.89674 LUMO: -0.09796 factor:1 | 1 (-0.08338) | 1 | 1 |
| G: -5717.87902 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.35272 HOMO: -7.02870 LUMO: 0.88709 factor:1 | 1 (-0.10800) | -1 | -1 |
| G: -5717.87902 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.38994 HOMO: -6.78380 LUMO: 0.22041 factor:1 | 1 (-0.14523) | -1 | -1 |
| G: -5717.87902 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.53755 HOMO: -7.24911 LUMO: -0.82178 factor:1 | -1 (0.70717) | 1 | 1 |
| G: -5717.87902 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.43038 HOMO: -6.77019 LUMO: 0.52790 factor:1 | 1 (-0.18566) | -1 | -1 |
| G: -5717.87902 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.12558 HOMO: -8.56070 LUMO: -1.83405 factor:1 | -1 (0.11913) | -1 | -1 |
| G: -5717.87902 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.97149 HOMO: -7.74164 LUMO: -2.36195 factor:1 | -1 (1.27322) | -1 | -1 |
| G: -5717.87902 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11979.78037 HOMO: -7.39878 LUMO: -2.41637 factor:1 | -1 (2.46434) | -1 | -1 |
| G: -5717.87902 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.31753 HOMO: -7.61647 LUMO: -2.34018 factor:1 | 1 (-0.07282) | -1 | -1 |
| G: -5717.87902 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.20474 HOMO: -6.93346 LUMO: -0.57688 factor:1 | -1 (0.03997) | -1 | -1 |
| G: -5717.87902 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.94087 HOMO: -6.85183 LUMO: -1.00410 factor:1 | -1 (0.30384) | -1 | -1 |
| G: -5717.87902 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.44445 HOMO: -7.18925 LUMO: -1.12655 factor:1 | 1 (-0.19973) | 1 | 1 |
| G: -5717.87902 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.50320 HOMO: -6.85183 LUMO: -1.60275 factor:1 | 1 (-0.25848) | -1 | -1 |
| G: -5717.87902 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.11408 HOMO: -7.51578 LUMO: 0.12517 factor:1 | -1 (1.13063) | 1 | 1 |
| G: -5717.87902 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.27435 HOMO: -7.36068 LUMO: 0.05714 factor:1 | 1 (-0.02963) | 1 | 1 |
| G: -5717.87902 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.01315 HOMO: -7.49674 LUMO: 0.18776 factor:1 | -1 (0.23157) | 1 | 1 |
| G: -5717.87902 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11979.67087 HOMO: -7.09401 LUMO: -1.24900 factor:1 | -1 (2.57384) | 1 | 1 |
| G: -5717.87902 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11979.72987 HOMO: -7.22462 LUMO: -1.61364 factor:1 | -1 (2.51485) | -1 | -1 |
| G: -5717.87902 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11979.53827 HOMO: -7.74436 LUMO: -0.18776 factor:1 | -1 (2.70644) | 1 | 1 |
| G: -5717.87902 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.04149 HOMO: -7.35252 LUMO: 0.75376 factor:1 | -1 (2.20322) | 1 | 1 |
| G: -5717.87902 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11979.88181 HOMO: -7.75252 LUMO: 0.00816 factor:1 | -1 (2.36290) | 1 | 1 |
| G: -5717.87902 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.98027 HOMO: -7.06680 LUMO: 0.24490 factor:1 | -1 (0.26444) | 1 | 1 |
| G: -5717.87902 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.98447 HOMO: -7.49129 LUMO: 0.14150 factor:1 | -1 (1.26024) | 1 | 1 |
| G: -5717.87902 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.79089 HOMO: -6.90625 LUMO: -1.11295 factor:1 | -1 (1.45382) | -1 | -1 |
| G: -5717.87902 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.91518 HOMO: -6.78380 LUMO: -0.93063 factor:1 | -1 (0.32953) | -1 | -1 |
| G: -5717.87902 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.01816 HOMO: -7.79878 LUMO: 0.30477 factor:1 | -1 (1.22655) | 1 | 1 |
| G: -5717.87902 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.66499 HOMO: -7.87498 LUMO: 0.61770 factor:1 | -1 (1.57973) | 1 | 1 |
| G: -5717.87902 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.66623 HOMO: -7.23823 LUMO: 0.30205 factor:1 | -1 (0.57849) | 1 | 1 |
| G: -5717.87902 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.71750 HOMO: -7.67633 LUMO: 0.13061 factor:1 | -1 (1.52721) | 1 | 1 |
| G: -5717.87902 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.42743 HOMO: -7.79606 LUMO: 0.34558 factor:1 | -1 (1.81729) | 1 | 1 |
| G: -5717.87902 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11979.85928 HOMO: -6.66135 LUMO: -2.60141 factor:1 | -1 (2.38543) | -1 | -1 |
| G: -5717.87902 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.19028 HOMO: -7.03142 LUMO: 0.50885 factor:1 | -1 (2.05443) | -1 | -1 |
| G: -5717.87902 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11979.97352 HOMO: -7.05591 LUMO: -0.06531 factor:1 | -1 (2.27120) | -1 | -1 |
| G: -5717.87902 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11979.90845 HOMO: -7.45592 LUMO: -1.39594 factor:1 | -1 (2.33626) | 1 | 1 |
| G: -5717.87902 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.10263 HOMO: -7.22462 LUMO: -1.10478 factor:1 | -1 (2.14208) | 1 | 1 |
| G: -5717.87902 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.15379 HOMO: -8.14709 LUMO: -0.55783 factor:1 | -1 (2.09092) | 1 | 1 |
| G: -5717.87902 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.31194 HOMO: -7.22190 LUMO: -1.14560 factor:1 | -1 (1.93277) | 1 | 1 |
| G: -5717.87902 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.68087 HOMO: -7.28721 LUMO: -1.14016 factor:1 | -1 (0.56385) | 1 | 1 |
| G: -5717.87902 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.39354 HOMO: -6.97156 LUMO: 0.51702 factor:1 | -1 (0.85117) | -1 | -1 |
| G: -5717.87902 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.91663 HOMO: -7.37156 LUMO: 0.29388 factor:1 | -1 (0.32809) | 1 | -1 |
| G: -5717.87902 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.00008 HOMO: -7.66273 LUMO: -1.59731 factor:1 | -1 (0.24463) | -1 | -1 |
| G: -5717.87902 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.00077 HOMO: -7.50490 LUMO: -1.49935 factor:1 | -1 (1.24394) | -1 | -1 |
| G: -5717.87902 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.01283 HOMO: -7.61102 LUMO: -1.45581 factor:1 | -1 (1.23189) | 1 | 1 |
| G: -5717.87902 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11983.06585 HOMO: -7.58653 LUMO: -1.61091 factor:1 | 1 (-0.82113) | -1 | -1 |
| G: -5717.87902 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.37936 HOMO: -7.36068 LUMO: -1.14560 factor:1 | 1 (-0.13464) | 1 | 1 |
| G: -5717.87902 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11983.02944 HOMO: -6.96339 LUMO: 0.26939 factor:1 | 1 (-0.78472) | -1 | -1 |
| G: -5717.87902 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.25503 HOMO: -6.53617 LUMO: 0.22313 factor:1 | 1 (-0.01031) | -1 | -1 |
| G: -5717.87902 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11983.39333 HOMO: -7.33619 LUMO: -1.02587 factor:1 | 1 (-1.14862) | 1 | 1 |
| G: -5717.87902 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.12232 HOMO: -6.87904 LUMO: 0.33742 factor:1 | -1 (0.12240) | -1 | -1 |
| G: -5717.87902 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.64478 HOMO: -6.88448 LUMO: 0.58777 factor:1 | 1 (-0.40006) | -1 | -1 |
| G: -5717.87902 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.75346 HOMO: -6.55522 LUMO: -1.51295 factor:1 | 1 (-0.50874) | -1 | -1 |
| G: -5717.87902 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.06194 HOMO: -7.43415 LUMO: 0.10612 factor:1 | -1 (0.18278) | 1 | 1 |
| G: -5717.87902 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.79706 HOMO: -7.54300 LUMO: -0.02449 factor:1 | -1 (0.44765) | 1 | 1 |
| G: -5717.87902 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.71747 HOMO: -7.42054 LUMO: 0.28028 factor:1 | -1 (0.52725) | 1 | 1 |
| G: -5717.87902 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.61591 HOMO: -6.98244 LUMO: -0.95784 factor:1 | -1 (0.62880) | -1 | -1 |
| G: -5717.87902 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.84937 HOMO: -6.96884 LUMO: -1.12383 factor:1 | -1 (1.39535) | -1 | -1 |
| G: -5717.87902 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11979.26923 HOMO: -6.80829 LUMO: -0.98233 factor:1 | -1 (2.97548) | -1 | -1 |
| G: -5717.87902 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11978.96710 HOMO: -7.60830 LUMO: 0.58504 factor:1 | -1 (3.27761) | 1 | 1 |
| G: -5717.87902 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11979.01897 HOMO: -7.52123 LUMO: 0.08163 factor:1 | -1 (3.22575) | 1 | 1 |
| G: -5717.87902 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11979.89972 HOMO: -7.59742 LUMO: 0.00272 factor:1 | -1 (2.34500) | 1 | 1 |
| G: -5717.87902 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11979.88905 HOMO: -6.99333 LUMO: -1.33880 factor:1 | -1 (2.35566) | -1 | -1 |
| G: -5717.87902 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11979.70486 HOMO: -6.63958 LUMO: -1.39322 factor:1 | -1 (2.53986) | -1 | -1 |
| G: -5717.87902 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11979.77242 HOMO: -7.86137 LUMO: 0.01633 factor:1 | -1 (2.47229) | 1 | 1 |
| G: -5717.87902 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11979.65275 HOMO: -7.29537 LUMO: 0.14694 factor:1 | -1 (2.59197) | 1 | 1 |
| G: -5717.87902 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11979.95175 HOMO: -6.95523 LUMO: 0.48708 factor:1 | -1 (2.29297) | -1 | -1 |
| G: -5717.87902 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.04530 HOMO: -7.10217 LUMO: -1.10478 factor:1 | -1 (2.19941) | 1 | 1 |
| G: -5717.87902 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11979.92524 HOMO: -6.88176 LUMO: -0.96328 factor:1 | -1 (2.31947) | -1 | -1 |
| G: -5717.87902 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.16481 HOMO: -7.89130 LUMO: -0.13334 factor:1 | -1 (2.07990) | 1 | 1 |
| G: -5717.87902 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.65252 HOMO: -7.75252 LUMO: 0.25579 factor:1 | -1 (1.59219) | 1 | 1 |
| G: -5717.87902 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11979.70279 HOMO: -6.87632 LUMO: -0.93063 factor:1 | -1 (2.54192) | -1 | -1 |
| G: -5717.87902 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11979.75961 HOMO: -6.78108 LUMO: -0.86804 factor:1 | -1 (2.48511) | -1 | -1 |
| G: -5717.87902 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11979.67729 HOMO: -5.98106 LUMO: 0.10340 factor:1 | -1 (2.56742) | -1 | -1 |
| G: -5717.87902 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11979.33416 HOMO: -6.40284 LUMO: -0.87349 factor:1 | -1 (2.91056) | -1 | -1 |
| G: -5717.87902 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11979.40662 HOMO: -6.77019 LUMO: -1.20819 factor:1 | -1 (2.83809) | -1 | -1 |
| G: -5717.87902 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.43777 HOMO: -6.90081 LUMO: -1.00682 factor:1 | -1 (1.80694) | -1 | -1 |
| G: -5717.87902 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11979.03478 HOMO: -6.59060 LUMO: -0.26667 factor:1 | -1 (3.20994) | -1 | -1 |
| G: -5717.87902 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11979.31990 HOMO: -6.50896 LUMO: -0.48708 factor:1 | -1 (2.92482) | -1 | -1 |
| G: -5717.87902 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11979.01309 HOMO: -6.20420 LUMO: -0.73471 factor:1 | -1 (3.23162) | -1 | -1 |
| G: -5717.87902 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11979.06150 HOMO: -6.17154 LUMO: -0.68573 factor:1 | -1 (3.18322) | -1 | -1 |
| G: -5717.87902 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11978.80016 HOMO: -6.21236 LUMO: 0.09796 factor:1 | -1 (3.44455) | -1 | -1 |
| G: -5717.87902 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11978.86735 HOMO: -6.38379 LUMO: 0.58232 factor:1 | -1 (3.37737) | -1 | -1 |
| G: -5717.87902 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11978.85516 HOMO: -7.42871 LUMO: 0.40273 factor:1 | -1 (3.38956) | 1 | 1 |
| G: -5717.87902 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.38182 HOMO: -6.54978 LUMO: 0.26395 factor:1 | -1 (1.86289) | -1 | -1 |
| G: -5717.87902 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.26658 HOMO: -7.14027 LUMO: 0.14150 factor:1 | -1 (1.97813) | 1 | 1 |
| G: -5717.87902 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.24261 HOMO: -7.25456 LUMO: -0.15783 factor:1 | -1 (2.00210) | 1 | 1 |
| G: -5717.87902 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.44025 HOMO: -6.90897 LUMO: 0.63403 factor:1 | -1 (1.80447) | -1 | -1 |
| G: -5717.87902 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.19684 HOMO: -6.49264 LUMO: 0.71022 factor:1 | -1 (2.04787) | -1 | -1 |
| G: -5717.87902 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.07523 HOMO: -6.56067 LUMO: -1.03947 factor:1 | -1 (2.16948) | -1 | -1 |
| G: -5717.87902 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.16827 HOMO: -6.79196 LUMO: -1.12655 factor:1 | -1 (2.07645) | -1 | -1 |
| G: -5717.87902 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11979.96650 HOMO: -6.95251 LUMO: -1.09118 factor:1 | -1 (2.27822) | -1 | -1 |
| G: -5717.87902 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11979.74962 HOMO: -7.47225 LUMO: -0.22041 factor:1 | -1 (2.49509) | 1 | 1 |
| G: -5717.87902 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11979.73392 HOMO: -7.13483 LUMO: -0.98505 factor:1 | -1 (2.51079) | 1 | 1 |
| G: -5717.87902 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11979.43971 HOMO: -6.99061 LUMO: -1.05852 factor:1 | -1 (2.80500) | -1 | -1 |
| G: -5717.87902 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11979.84878 HOMO: -6.52257 LUMO: -1.11022 factor:1 | -1 (2.39594) | -1 | -1 |
| G: -5717.87902 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11979.88611 HOMO: -6.75114 LUMO: -1.09934 factor:1 | -1 (2.35860) | -1 | -1 |
| G: -5717.87902 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.75073 HOMO: -6.82189 LUMO: -0.89253 factor:1 | -1 (1.49399) | -1 | -1 |
| G: -5717.87902 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.43265 HOMO: -6.83278 LUMO: -0.97961 factor:1 | -1 (1.81206) | -1 | -1 |
| G: -5717.87902 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.89397 HOMO: -6.65318 LUMO: -0.84355 factor:1 | -1 (1.35075) | -1 | -1 |
| G: -5717.87902 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.88548 HOMO: -6.75931 LUMO: -0.88437 factor:1 | -1 (1.35924) | -1 | -1 |
| G: -5717.87902 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.84210 HOMO: -6.19059 LUMO: -0.45715 factor:1 | -1 (1.40261) | -1 | -1 |
| G: -5717.87902 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.20570 HOMO: -7.09673 LUMO: -2.01908 factor:1 | -1 (1.03901) | -1 | -1 |
| G: -5717.87902 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.64343 HOMO: -7.88042 LUMO: 0.38640 factor:1 | -1 (1.60128) | 1 | 1 |
| G: -5717.87902 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11979.49666 HOMO: -7.83144 LUMO: 0.14422 factor:1 | -1 (2.74805) | 1 | 1 |
| G: -5717.87902 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11979.39887 HOMO: -7.46408 LUMO: 0.44627 factor:1 | -1 (2.84585) | 1 | 1 |
| G: -5717.87902 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.03648 HOMO: -7.12394 LUMO: -2.04902 factor:1 | -1 (2.20823) | -1 | -1 |
| G: -5717.87902 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.15679 HOMO: -6.78380 LUMO: -1.11295 factor:1 | -1 (2.08793) | -1 | -1 |
| G: -5717.87902 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.43635 HOMO: -7.12938 LUMO: -0.23674 factor:1 | -1 (1.80836) | 1 | 1 |
| G: -5717.87902 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.52548 HOMO: -6.14705 LUMO: -0.20409 factor:1 | 1 (-0.28077) | -1 | -1 |
| G: -5717.87902 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.29761 HOMO: -6.50080 LUMO: -0.28300 factor:1 | 1 (-0.05290) | -1 | -1 |
| G: -5717.87902 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.02011 HOMO: -6.50352 LUMO: -0.62042 factor:1 | -1 (0.22460) | -1 | -1 |
| G: -5717.87902 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.08825 HOMO: -6.46543 LUMO: -0.53879 factor:1 | -1 (0.15647) | -1 | -1 |
| G: -5717.87902 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.39873 HOMO: -7.32803 LUMO: -0.52790 factor:1 | 1 (-0.15402) | 1 | 1 |
| G: -5717.87902 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.82871 HOMO: -5.94025 LUMO: -0.17687 factor:1 | -1 (0.41601) | -1 | -1 |
| G: -5717.87902 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.51699 HOMO: -5.62187 LUMO: 0.05714 factor:1 | 1 (-0.27228) | -1 | -1 |
| G: -5717.87902 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.96196 HOMO: -7.03414 LUMO: -1.04492 factor:1 | -1 (0.28275) | -1 | -1 |
| G: -5717.87902 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.55297 HOMO: -6.75387 LUMO: -2.02181 factor:1 | 1 (-0.30825) | -1 | -1 |
| G: -5717.87902 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.32850 HOMO: -6.55250 LUMO: -0.75648 factor:1 | 1 (-0.08378) | -1 | -1 |
| G: -5717.87902 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.75031 HOMO: -6.81101 LUMO: -1.02043 factor:1 | -1 (0.49440) | -1 | -1 |
| G: -5717.87902 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.37098 HOMO: -6.69672 LUMO: -2.81910 factor:1 | 1 (-0.12626) | -1 | -1 |
| G: -5717.87902 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.10224 HOMO: -6.69128 LUMO: -2.58236 factor:1 | -1 (0.14248) | -1 | -1 |
| G: -5717.87902 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.81483 HOMO: -6.73482 LUMO: -2.06807 factor:1 | -1 (0.42989) | -1 | -1 |
| G: -5717.87902 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.52693 HOMO: -7.66545 LUMO: 0.17143 factor:1 | -1 (0.71778) | 1 | 1 |
| G: -5717.87902 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.28066 HOMO: -6.87904 LUMO: -1.25172 factor:1 | 1 (-0.03595) | -1 | -1 |
| G: -5717.87902 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.33770 HOMO: -6.84366 LUMO: -0.19320 factor:1 | 1 (-0.09298) | -1 | -1 |
| G: -5717.87902 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.43088 HOMO: -6.97972 LUMO: -0.97961 factor:1 | -1 (0.81384) | -1 | -1 |
| G: -5717.87902 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.35941 HOMO: -6.72121 LUMO: -0.70477 factor:1 | 1 (-0.11470) | -1 | -1 |
| G: -5717.87902 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11983.00525 HOMO: -7.18925 LUMO: 0.40001 factor:1 | 1 (-0.76053) | 1 | 1 |
| G: -5717.87902 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.96418 HOMO: -6.72121 LUMO: 0.19592 factor:1 | 1 (-0.71947) | -1 | -1 |
| G: -5717.87902 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.32714 HOMO: -6.85999 LUMO: -0.39457 factor:1 | 1 (-0.08242) | -1 | -1 |
| G: -5717.87902 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11983.08693 HOMO: -6.90625 LUMO: 0.05987 factor:1 | 1 (-0.84222) | -1 | -1 |
| G: -5717.87902 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11983.51486 HOMO: -7.00421 LUMO: 0.37552 factor:1 | 1 (-1.27015) | -1 | -1 |
| G: -5717.87902 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.41680 HOMO: -6.56883 LUMO: -0.97689 factor:1 | 1 (-0.17208) | -1 | -1 |
| G: -5717.87902 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.71754 HOMO: -6.66679 LUMO: 0.56055 factor:1 | 1 (-0.47283) | -1 | -1 |
| G: -5717.87902 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11983.53263 HOMO: -6.75931 LUMO: 0.32926 factor:1 | 1 (-1.28791) | -1 | -1 |
| G: -5717.87902 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.10830 HOMO: -6.53617 LUMO: -1.06397 factor:1 | -1 (0.13641) | -1 | -1 |
| G: -5717.87902 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.17473 HOMO: -6.78108 LUMO: 0.42722 factor:1 | -1 (0.06999) | -1 | -1 |
| G: -5717.87902 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.85550 HOMO: -7.05319 LUMO: 0.61498 factor:1 | 1 (-0.61079) | -1 | -1 |
| G: -5717.87902 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.46603 HOMO: -6.78380 LUMO: 1.49391 factor:1 | 1 (-0.22131) | -1 | -1 |
| G: -5717.87902 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.68269 HOMO: -7.21102 LUMO: 0.27211 factor:1 | -1 (0.56202) | 1 | 1 |
| G: -5717.87902 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.61436 HOMO: -6.67223 LUMO: 0.81362 factor:1 | -1 (0.63035) | -1 | -1 |
| G: -5717.87902 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.66895 HOMO: -6.69944 LUMO: 1.40683 factor:1 | -1 (0.57577) | -1 | -1 |
| G: -5717.87902 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.50654 HOMO: -7.02598 LUMO: 1.46941 factor:1 | 1 (-0.26183) | -1 | -1 |
| G: -5717.87902 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.25142 HOMO: -5.85045 LUMO: -0.76736 factor:1 | -1 (0.99330) | -1 | -1 |
| G: -5717.87902 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.45675 HOMO: -6.53890 LUMO: -0.50885 factor:1 | 1 (-0.21203) | -1 | -1 |
| G: -5717.87902 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.51364 HOMO: -6.42733 LUMO: -0.63947 factor:1 | 1 (-0.26893) | -1 | -1 |
| G: -5717.87902 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11983.13080 HOMO: -6.82189 LUMO: -0.85444 factor:1 | 1 (-0.88608) | -1 | -1 |
| G: -5717.87902 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.40047 HOMO: -6.97428 LUMO: -1.22179 factor:1 | 1 (-0.15576) | -1 | -1 |
| G: -5717.87902 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11983.11896 HOMO: -6.93346 LUMO: -1.09934 factor:1 | 1 (-0.87425) | -1 | -1 |
| G: -5717.87902 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.47748 HOMO: -7.17292 LUMO: -1.11839 factor:1 | 1 (-0.23277) | 1 | 1 |
| G: -5717.87902 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11983.18351 HOMO: -7.00965 LUMO: -1.23268 factor:1 | 1 (-0.93879) | -1 | -1 |
| G: -5717.87902 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11983.46452 HOMO: -6.73210 LUMO: -1.12383 factor:1 | 1 (-1.21980) | -1 | -1 |
| G: -5717.87902 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.64412 HOMO: -7.61375 LUMO: -0.11973 factor:1 | 1 (-0.39941) | 1 | 1 |
| G: -5717.87902 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.07777 HOMO: -7.42327 LUMO: 0.41906 factor:1 | -1 (0.16694) | 1 | 1 |
| G: -5717.87902 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.93493 HOMO: -6.94162 LUMO: -1.01771 factor:1 | 1 (-0.69022) | -1 | -1 |
| G: -5717.87902 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.45544 HOMO: -6.82189 LUMO: -0.92791 factor:1 | 1 (-0.21072) | -1 | -1 |
| G: -5717.87902 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.76845 HOMO: -6.92258 LUMO: -1.73881 factor:1 | 1 (-0.52374) | -1 | -1 |
| G: -5717.87902 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.34209 HOMO: -6.50896 LUMO: -1.60819 factor:1 | -1 (1.90262) | -1 | -1 |
| G: -5717.87902 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.14998 HOMO: -6.38379 LUMO: -2.18780 factor:1 | -1 (2.09473) | -1 | -1 |
| G: -5717.87902 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.27535 HOMO: -6.48992 LUMO: -0.97417 factor:1 | -1 (1.96937) | -1 | -1 |
| G: -5717.87902 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.04841 HOMO: -6.01644 LUMO: -0.04354 factor:1 | -1 (0.19630) | -1 | -1 |
| G: -5717.87902 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.10687 HOMO: -6.70761 LUMO: -0.14422 factor:1 | -1 (1.13784) | -1 | -1 |
| G: -5717.87902 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.78099 HOMO: -6.70216 LUMO: 0.14422 factor:1 | -1 (1.46373) | -1 | -1 |
| G: -5717.87902 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.78872 HOMO: -7.07224 LUMO: -0.10885 factor:1 | -1 (1.45600) | 1 | 1 |
| G: -5717.87902 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.06184 HOMO: -7.52667 LUMO: -0.74287 factor:1 | -1 (1.18288) | 1 | 1 |
| G: -5717.87902 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.82300 HOMO: -6.48447 LUMO: -0.96056 factor:1 | -1 (1.42171) | -1 | -1 |
| G: -5717.87902 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.92940 HOMO: -6.22597 LUMO: -0.41361 factor:1 | -1 (1.31532) | -1 | -1 |
| G: -5717.87902 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.67475 HOMO: -6.12256 LUMO: -1.05852 factor:1 | -1 (1.56996) | -1 | -1 |
| G: -5717.87902 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.03318 HOMO: -6.97428 LUMO: -0.60681 factor:1 | -1 (1.21153) | -1 | -1 |
| G: -5717.87902 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.61367 HOMO: -6.78380 LUMO: -0.88981 factor:1 | 1 (-0.36896) | -1 | -1 |
| G: -5717.87902 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11983.24468 HOMO: -6.85999 LUMO: 0.07891 factor:1 | 1 (-0.99996) | -1 | -1 |
| G: -5717.87902 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.64848 HOMO: -7.08312 LUMO: -0.60137 factor:1 | 1 (-0.40376) | 1 | 1 |
| G: -5717.87902 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11983.51290 HOMO: -6.57699 LUMO: -0.68028 factor:1 | 1 (-1.26819) | -1 | -1 |
| G: -5717.87902 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11983.06775 HOMO: -6.09807 LUMO: -0.31837 factor:1 | 1 (-0.82304) | -1 | -1 |
| G: -5717.87902 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.86095 HOMO: -6.10624 LUMO: 0.14966 factor:1 | -1 (0.38376) | -1 | -1 |
| G: -5717.87902 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.79950 HOMO: -6.77019 LUMO: -0.95784 factor:1 | 1 (-0.55479) | -1 | -1 |
| G: -5717.87902 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.83267 HOMO: -5.93208 LUMO: -0.44627 factor:1 | 1 (-0.58796) | -1 | -1 |
| G: -5717.87902 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.18322 HOMO: -6.12256 LUMO: -0.27756 factor:1 | -1 (0.06150) | -1 | -1 |
| G: -5717.87902 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.54146 HOMO: -5.98106 LUMO: -0.37824 factor:1 | -1 (0.70325) | -1 | -1 |
| G: -5717.87902 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.26629 HOMO: -7.06408 LUMO: -1.12927 factor:1 | 1 (-0.02158) | 1 | 1 |
| G: -5717.87902 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.12188 HOMO: -6.70761 LUMO: -0.98505 factor:1 | -1 (0.12283) | -1 | -1 |
| G: -5717.87902 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.39895 HOMO: -7.00965 LUMO: -0.42722 factor:1 | 1 (-0.15423) | -1 | -1 |
| G: -5717.87902 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.52001 HOMO: -5.96201 LUMO: -0.59049 factor:1 | 1 (-0.27530) | -1 | -1 |
| G: -5717.87902 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.90072 HOMO: -6.34570 LUMO: -1.68438 factor:1 | -1 (1.34400) | -1 | -1 |
| G: -5717.87902 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.10628 HOMO: -6.97156 LUMO: -1.85854 factor:1 | -1 (2.13843) | -1 | -1 |
| G: -5717.87902 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.19304 HOMO: -5.91848 LUMO: -2.51433 factor:1 | -1 (0.05167) | -1 | -1 |
| G: -5717.87902 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.94844 HOMO: -6.39195 LUMO: -1.66262 factor:1 | -1 (0.29628) | -1 | -1 |
| G: -5717.87902 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.31106 HOMO: -6.50352 LUMO: 0.19592 factor:1 | 1 (-0.06634) | -1 | -1 |
| G: -5717.87902 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11979.68772 HOMO: -6.45998 LUMO: 0.34831 factor:1 | -1 (2.55700) | -1 | -1 |
| G: -5717.87902 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.30307 HOMO: -7.05319 LUMO: 0.23402 factor:1 | -1 (1.94164) | -1 | -1 |
| G: -5717.87902 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.89962 HOMO: -6.61237 LUMO: 0.18232 factor:1 | -1 (0.34509) | -1 | -1 |
| G: -5717.87902 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.23607 HOMO: -6.57427 LUMO: 0.40545 factor:1 | -1 (1.00864) | -1 | -1 |
| G: -5717.87902 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.12532 HOMO: -7.26544 LUMO: 0.41089 factor:1 | -1 (1.11939) | 1 | 1 |
| G: -5717.87902 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.79687 HOMO: -6.26406 LUMO: -0.85444 factor:1 | -1 (0.44784) | -1 | -1 |
| G: -5717.87902 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.61635 HOMO: -6.25318 LUMO: -0.79457 factor:1 | -1 (0.62837) | -1 | -1 |
| G: -5717.87902 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.37547 HOMO: -6.68040 LUMO: 0.41089 factor:1 | 1 (-0.13075) | -1 | -1 |
| G: -5717.87902 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.04887 HOMO: -6.37835 LUMO: 0.37280 factor:1 | -1 (0.19584) | -1 | -1 |
| G: -5717.87902 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.64721 HOMO: -6.56067 LUMO: 0.62858 factor:1 | -1 (0.59751) | -1 | -1 |
| G: -5717.87902 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.83146 HOMO: -6.74026 LUMO: -0.04082 factor:1 | -1 (0.41326) | -1 | -1 |
| G: -5717.87902 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.01462 HOMO: -6.53617 LUMO: 0.35103 factor:1 | -1 (1.23009) | -1 | -1 |
| G: -5717.87902 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.71372 HOMO: -6.51985 LUMO: 0.25851 factor:1 | -1 (1.53099) | -1 | -1 |
| G: -5717.87902 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.99007 HOMO: -6.58788 LUMO: -1.98371 factor:1 | -1 (0.25464) | -1 | -1 |
| G: -5717.87902 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.15313 HOMO: -6.51441 LUMO: 0.29116 factor:1 | -1 (1.09158) | -1 | -1 |
| G: -5717.87902 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.91930 HOMO: -6.81101 LUMO: 0.35647 factor:1 | -1 (1.32541) | -1 | -1 |
| G: -5717.87902 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.46018 HOMO: -6.42733 LUMO: 0.10340 factor:1 | -1 (0.78453) | -1 | -1 |
| G: -5717.87902 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.00413 HOMO: -6.70761 LUMO: 0.28028 factor:1 | -1 (2.24059) | -1 | -1 |
| G: -5717.87902 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.24869 HOMO: -6.67495 LUMO: 0.01633 factor:1 | 1 (-0.00397) | -1 | -1 |
| G: -5717.87902 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.57152 HOMO: -6.75387 LUMO: 0.15510 factor:1 | 1 (-0.32681) | -1 | -1 |
| G: -5717.87902 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.53686 HOMO: -6.56067 LUMO: 0.35919 factor:1 | 1 (-0.29214) | -1 | -1 |
| G: -5717.87902 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.60246 HOMO: -7.16748 LUMO: 0.21497 factor:1 | 1 (-0.35775) | 1 | 1 |
| G: -5717.87902 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.30465 HOMO: -6.71849 LUMO: 0.26667 factor:1 | -1 (1.94006) | -1 | -1 |
| G: -5717.87902 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.15445 HOMO: -6.69128 LUMO: 0.55783 factor:1 | -1 (0.09026) | -1 | -1 |
| G: -5717.87902 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.27216 HOMO: -6.71305 LUMO: 0.45987 factor:1 | -1 (1.97255) | -1 | -1 |
| G: -5717.87902 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.32196 HOMO: -5.90487 LUMO: -0.70750 factor:1 | -1 (1.92276) | -1 | -1 |
| G: -5717.87902 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11979.96241 HOMO: -6.84638 LUMO: -0.72110 factor:1 | -1 (2.28230) | -1 | -1 |
| G: -5717.87902 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.22947 HOMO: -6.66135 LUMO: -1.13471 factor:1 | -1 (2.01525) | -1 | -1 |
| G: -5717.87902 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.03894 HOMO: -6.74026 LUMO: -0.64763 factor:1 | -1 (0.20577) | -1 | -1 |
| G: -5717.87902 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.09729 HOMO: -6.69672 LUMO: -1.05036 factor:1 | -1 (1.14742) | -1 | -1 |
| G: -5717.87902 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.16352 HOMO: -6.78924 LUMO: -1.03675 factor:1 | -1 (1.08119) | -1 | -1 |
| G: -5717.87902 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.73205 HOMO: -6.81373 LUMO: -0.85988 factor:1 | -1 (0.51266) | -1 | -1 |
| G: -5717.87902 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.89405 HOMO: -7.26544 LUMO: 0.91158 factor:1 | -1 (1.35066) | 1 | 1 |
| G: -5717.87902 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.30859 HOMO: -6.64230 LUMO: -1.92929 factor:1 | -1 (0.93613) | -1 | -1 |
| G: -5717.87902 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.39118 HOMO: -7.20830 LUMO: 0.11429 factor:1 | -1 (0.85354) | 1 | 1 |
| G: -5717.87902 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.10927 HOMO: -7.17020 LUMO: 0.04898 factor:1 | -1 (1.13545) | 1 | 1 |
| G: -5717.87902 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.12770 HOMO: -7.16476 LUMO: 0.04898 factor:1 | -1 (2.11702) | 1 | 1 |
| G: -5717.87902 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.36756 HOMO: -6.59332 LUMO: -0.49253 factor:1 | -1 (1.87715) | -1 | -1 |
| G: -5717.87902 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.30612 HOMO: -7.46953 LUMO: 0.84083 factor:1 | -1 (1.93859) | 1 | 1 |
| G: -5717.87902 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.43853 HOMO: -7.39878 LUMO: 0.88709 factor:1 | -1 (1.80618) | 1 | 1 |
| G: -5717.87902 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.84012 HOMO: -6.84094 LUMO: -0.61498 factor:1 | -1 (1.40460) | -1 | -1 |
| G: -5717.87902 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.40884 HOMO: -6.03549 LUMO: -0.27211 factor:1 | -1 (0.83588) | -1 | -1 |
| G: -5717.87902 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.88765 HOMO: -7.31170 LUMO: -0.64763 factor:1 | -1 (0.35707) | 1 | 1 |
| G: -5717.87902 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.79105 HOMO: -6.88992 LUMO: -0.84627 factor:1 | -1 (0.45367) | -1 | -1 |
| G: -5717.87902 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.16259 HOMO: -7.12666 LUMO: -0.09252 factor:1 | -1 (0.08212) | 1 | 1 |
| G: -5717.87902 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.45735 HOMO: -6.70489 LUMO: -0.63675 factor:1 | -1 (0.78736) | -1 | -1 |
| G: -5717.87902 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.97929 HOMO: -6.98788 LUMO: 0.86804 factor:1 | -1 (0.26542) | -1 | -1 |
| G: -5717.87902 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.28172 HOMO: -6.80285 LUMO: -0.60954 factor:1 | 1 (-0.03701) | -1 | -1 |
| G: -5717.87902 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.29267 HOMO: -7.02054 LUMO: -0.74287 factor:1 | -1 (0.95204) | -1 | -1 |
| G: -5717.87902 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.83728 HOMO: -7.03686 LUMO: -0.81090 factor:1 | -1 (0.40744) | -1 | -1 |
| G: -5717.87902 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.19108 HOMO: -6.70489 LUMO: -1.00954 factor:1 | -1 (0.05363) | -1 | -1 |
| G: -5717.87902 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.83099 HOMO: -7.69810 LUMO: 0.00544 factor:1 | -1 (0.41372) | 1 | 1 |
| G: -5717.87902 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.12200 HOMO: -6.83550 LUMO: -0.11157 factor:1 | -1 (1.12271) | -1 | -1 |
| G: -5717.87902 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.86366 HOMO: -6.76203 LUMO: -2.13609 factor:1 | -1 (1.38106) | -1 | -1 |
| G: -5717.87902 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.28051 HOMO: -6.72121 LUMO: -2.62862 factor:1 | -1 (0.96421) | -1 | -1 |
| G: -5717.87902 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.99672 HOMO: -6.48719 LUMO: -2.73474 factor:1 | -1 (1.24800) | -1 | -1 |
| G: -5717.87902 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.72675 HOMO: -6.83006 LUMO: -0.00544 factor:1 | -1 (0.51797) | -1 | -1 |
| G: -5717.87902 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.39093 HOMO: -6.84094 LUMO: -1.11022 factor:1 | -1 (0.85378) | -1 | -1 |
| G: -5717.87902 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.18149 HOMO: -6.66951 LUMO: -1.23812 factor:1 | -1 (2.06322) | -1 | -1 |
| G: -5717.87902 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.20253 HOMO: -6.78380 LUMO: -1.27894 factor:1 | -1 (2.04219) | -1 | -1 |
| G: -5717.87902 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.29875 HOMO: -6.50352 LUMO: -0.56055 factor:1 | -1 (1.94597) | -1 | -1 |
| G: -5717.87902 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.17221 HOMO: -7.77974 LUMO: -0.26395 factor:1 | -1 (2.07250) | 1 | 1 |
| G: -5717.87902 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.22664 HOMO: -7.01510 LUMO: -1.64085 factor:1 | -1 (2.01808) | -1 | -1 |
| G: -5717.87902 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11979.87526 HOMO: -6.59876 LUMO: -0.91158 factor:1 | -1 (2.36946) | -1 | -1 |
| G: -5717.87902 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11979.88903 HOMO: -4.67219 LUMO: -0.67756 factor:1 | -1 (2.35569) | -1 | -1 |
| G: -5717.87902 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.13600 HOMO: -6.70489 LUMO: -0.65579 factor:1 | -1 (2.10872) | -1 | -1 |
| G: -5717.87902 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11979.73778 HOMO: -6.62325 LUMO: -0.60409 factor:1 | -1 (2.50693) | -1 | -1 |
| G: -5717.87902 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.12683 HOMO: -6.20147 LUMO: 0.15238 factor:1 | -1 (2.11789) | -1 | -1 |
| G: -5717.87902 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.04203 HOMO: -6.43549 LUMO: -0.07075 factor:1 | -1 (2.20268) | -1 | -1 |
| G: -5717.87902 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.46984 HOMO: -7.02054 LUMO: 0.13061 factor:1 | -1 (0.77487) | -1 | -1 |
| G: -5717.87902 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.95253 HOMO: -7.04503 LUMO: 0.30749 factor:1 | -1 (1.29219) | -1 | -1 |
| G: -5717.87902 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.09331 HOMO: -6.74842 LUMO: -0.99594 factor:1 | -1 (0.15140) | -1 | -1 |
| G: -5717.87902 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.70483 HOMO: -6.35658 LUMO: 0.41633 factor:1 | 1 (-0.46012) | -1 | -1 |
| G: -5717.87902 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.32668 HOMO: -6.79740 LUMO: 0.56872 factor:1 | 1 (-0.08196) | -1 | -1 |
| G: -5717.87902 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.40902 HOMO: -6.51713 LUMO: -0.05987 factor:1 | 1 (-0.16430) | -1 | -1 |
| G: -5717.87902 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.14711 HOMO: -6.68040 LUMO: 0.34558 factor:1 | -1 (0.09761) | -1 | -1 |
| G: -5717.87902 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.96074 HOMO: -6.39740 LUMO: 0.50069 factor:1 | -1 (0.28398) | -1 | -1 |
| G: -5717.87902 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.93230 HOMO: -6.91713 LUMO: -0.97145 factor:1 | -1 (0.31241) | -1 | -1 |
| G: -5717.87902 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.12300 HOMO: -7.10761 LUMO: -0.27483 factor:1 | -1 (0.12172) | 1 | -1 |
| G: -5717.87902 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.15949 HOMO: -6.98788 LUMO: 0.40273 factor:1 | -1 (0.08523) | -1 | -1 |
| G: -5717.87902 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11979.74698 HOMO: -6.87087 LUMO: 0.28572 factor:1 | -1 (2.49773) | -1 | -1 |
| G: -5717.87902 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.11374 HOMO: -7.36612 LUMO: -0.12245 factor:1 | -1 (2.13098) | 1 | 1 |
| G: -5717.87902 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11979.89542 HOMO: -6.72938 LUMO: 0.33742 factor:1 | -1 (2.34930) | -1 | -1 |
| G: -5717.87902 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.94317 HOMO: -7.32531 LUMO: 0.07619 factor:1 | -1 (1.30155) | 1 | 1 |
| G: -5717.87902 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.57146 HOMO: -6.87087 LUMO: -0.08436 factor:1 | -1 (1.67326) | -1 | -1 |
| G: -5717.87902 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.69875 HOMO: -6.67495 LUMO: 0.85988 factor:1 | -1 (0.54597) | -1 | -1 |
| G: -5717.87902 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.04055 HOMO: -6.96339 LUMO: 0.65307 factor:1 | -1 (0.20417) | -1 | -1 |
| G: -5717.87902 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.10399 HOMO: -6.58516 LUMO: -0.78641 factor:1 | -1 (1.14073) | -1 | -1 |
| G: -5717.87902 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.37006 HOMO: -6.56883 LUMO: 0.44355 factor:1 | -1 (0.87466) | -1 | -1 |
| G: -5717.87902 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.64827 HOMO: -6.68312 LUMO: 0.43538 factor:1 | -1 (0.59645) | -1 | -1 |
| G: -5717.87902 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.81274 HOMO: -6.81917 LUMO: 0.20681 factor:1 | -1 (1.43197) | -1 | -1 |
| G: -5717.87902 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.66275 HOMO: -6.91169 LUMO: 0.08163 factor:1 | -1 (1.58196) | -1 | -1 |
| G: -5717.87902 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.80773 HOMO: -4.88444 LUMO: -0.49253 factor:1 | -1 (0.43699) | -1 | -1 |
| G: -5717.87902 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.92156 HOMO: -6.42189 LUMO: 0.64763 factor:1 | -1 (1.32315) | -1 | -1 |
| G: -5717.87902 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.76295 HOMO: -6.24501 LUMO: 0.55783 factor:1 | -1 (1.48177) | -1 | -1 |
| G: -5717.87902 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.10423 HOMO: -6.41372 LUMO: 0.29388 factor:1 | -1 (1.14048) | -1 | -1 |
| G: -5717.87902 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11979.98827 HOMO: -5.67902 LUMO: 1.77690 factor:1 | -1 (2.25645) | -1 | -1 |
| G: -5717.87902 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.50585 HOMO: -6.55794 LUMO: 0.05170 factor:1 | -1 (1.73886) | -1 | -1 |
| G: -5717.87902 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.35295 HOMO: -6.52801 LUMO: 0.25851 factor:1 | -1 (1.89176) | -1 | -1 |
| G: -5717.87902 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.23926 HOMO: -7.08857 LUMO: 0.11157 factor:1 | -1 (2.00545) | 1 | 1 |
| G: -5717.87902 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11979.85400 HOMO: -6.58243 LUMO: 0.75648 factor:1 | -1 (2.39071) | -1 | -1 |
| G: -5717.87902 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.04895 HOMO: -7.22190 LUMO: 0.45171 factor:1 | -1 (2.19577) | 1 | 1 |
| G: -5717.87902 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.07540 HOMO: -6.47087 LUMO: 0.00000 factor:1 | -1 (2.16932) | -1 | -1 |
| G: -5717.87902 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.12315 HOMO: -6.78652 LUMO: 1.32247 factor:1 | -1 (2.12156) | -1 | -1 |
| G: -5717.87902 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.32751 HOMO: -6.74026 LUMO: 1.45309 factor:1 | -1 (1.91721) | -1 | -1 |
| G: -5717.87902 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.25374 HOMO: -6.69944 LUMO: 0.76464 factor:1 | -1 (1.99098) | -1 | -1 |
| G: -5717.87902 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.28196 HOMO: -6.62325 LUMO: 0.64763 factor:1 | -1 (1.96276) | -1 | -1 |
| G: -5717.87902 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11979.96933 HOMO: -6.45182 LUMO: 0.49253 factor:1 | -1 (2.27539) | -1 | -1 |
| G: -5717.87902 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.01798 HOMO: -7.14843 LUMO: 0.62586 factor:1 | -1 (2.22673) | 1 | 1 |
| G: -5717.87902 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11979.61593 HOMO: -6.87087 LUMO: 1.53200 factor:1 | -1 (2.62878) | -1 | -1 |
| G: -5717.87902 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11979.86053 HOMO: -6.54978 LUMO: 0.45171 factor:1 | -1 (2.38418) | -1 | -1 |
| G: -5717.87902 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.37486 HOMO: -6.63686 LUMO: 0.80001 factor:1 | -1 (1.86986) | -1 | -1 |
| G: -5717.87902 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.33045 HOMO: -7.00693 LUMO: 1.56193 factor:1 | -1 (1.91427) | -1 | -1 |
| G: -5717.87902 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.20933 HOMO: -6.02460 LUMO: 1.72792 factor:1 | -1 (2.03538) | -1 | -1 |
| G: -5717.87902 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.36833 HOMO: -6.36746 LUMO: -1.20002 factor:1 | -1 (1.87639) | -1 | -1 |
| G: -5717.87902 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11979.88965 HOMO: -7.26816 LUMO: -1.06397 factor:1 | -1 (2.35506) | 1 | 1 |
| G: -5717.87902 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11979.88761 HOMO: -7.34707 LUMO: -1.09662 factor:1 | -1 (2.35710) | 1 | 1 |
| G: -5717.87902 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.22250 HOMO: -7.93212 LUMO: -0.13606 factor:1 | -1 (2.02221) | 1 | 1 |
| G: -5717.87902 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.04984 HOMO: -6.80285 LUMO: 0.58504 factor:1 | -1 (2.19487) | -1 | -1 |
| G: -5717.87902 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.79949 HOMO: -7.12938 LUMO: 0.32926 factor:1 | -1 (1.44522) | 1 | -1 |
| G: -5717.87902 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.64286 HOMO: -6.86815 LUMO: -1.30070 factor:1 | -1 (1.60185) | -1 | -1 |
| G: -5717.87902 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.85389 HOMO: -6.99333 LUMO: -1.03947 factor:1 | -1 (1.39083) | -1 | -1 |
| G: -5717.87902 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.64202 HOMO: -7.56749 LUMO: -0.11157 factor:1 | -1 (1.60270) | 1 | 1 |
| G: -5717.87902 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.29847 HOMO: -7.57293 LUMO: -0.07891 factor:1 | -1 (1.94624) | 1 | 1 |
| G: -5717.87902 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.33431 HOMO: -7.30626 LUMO: 0.27211 factor:1 | -1 (1.91040) | 1 | 1 |
| G: -5717.87902 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.44295 HOMO: -7.77974 LUMO: 0.27211 factor:1 | 1 (-0.19823) | 1 | 1 |
| G: -5717.87902 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.44409 HOMO: -7.11578 LUMO: 0.19864 factor:1 | 1 (-0.19938) | 1 | 1 |
| G: -5717.87902 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.41664 HOMO: -7.71171 LUMO: 0.57688 factor:1 | 1 (-0.17192) | 1 | 1 |
| G: -5717.87902 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.17894 HOMO: -7.83688 LUMO: 0.37824 factor:1 | -1 (0.06577) | 1 | 1 |
| G: -5717.87902 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.13870 HOMO: -6.94979 LUMO: -1.66534 factor:1 | -1 (0.10602) | -1 | -1 |
| G: -5717.87902 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.19704 HOMO: -6.97156 LUMO: -1.13199 factor:1 | -1 (0.04767) | -1 | -1 |
| G: -5717.87902 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.23413 HOMO: -6.91441 LUMO: -1.08301 factor:1 | -1 (0.01059) | -1 | -1 |
| G: -5717.87902 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.09312 HOMO: -6.71849 LUMO: -0.74831 factor:1 | -1 (0.15159) | -1 | -1 |
| G: -5717.87902 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.14120 HOMO: -7.09401 LUMO: -1.77690 factor:1 | -1 (0.10351) | -1 | -1 |
| G: -5717.87902 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.15372 HOMO: -6.97156 LUMO: -1.45037 factor:1 | -1 (0.09099) | -1 | -1 |
| G: -5717.87902 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.01472 HOMO: -7.22462 LUMO: -1.11295 factor:1 | -1 (0.22999) | 1 | 1 |
| G: -5717.87902 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.95388 HOMO: -7.85321 LUMO: 0.16599 factor:1 | -1 (0.29084) | 1 | 1 |
| G: -5717.87902 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.16817 HOMO: -7.71987 LUMO: 0.55511 factor:1 | -1 (0.07655) | 1 | 1 |
| G: -5717.87902 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.84536 HOMO: -7.63551 LUMO: 0.14422 factor:1 | -1 (0.39935) | 1 | 1 |
| G: -5717.87902 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.02536 HOMO: -6.98788 LUMO: -0.80546 factor:1 | -1 (0.21935) | -1 | -1 |
| G: -5717.87902 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.95534 HOMO: -6.98788 LUMO: -1.16737 factor:1 | 1 (-0.71063) | -1 | -1 |
| G: -5717.87902 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.19416 HOMO: -6.56611 LUMO: -1.60819 factor:1 | -1 (0.05056) | -1 | -1 |
| G: -5717.87902 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11983.01357 HOMO: -6.95251 LUMO: 0.66396 factor:1 | 1 (-0.76886) | -1 | -1 |
| G: -5717.87902 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.31808 HOMO: -7.35252 LUMO: 0.49797 factor:1 | 1 (-0.07336) | 1 | 1 |
| G: -5717.87902 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.85115 HOMO: -6.90897 LUMO: -0.81090 factor:1 | 1 (-0.60643) | -1 | -1 |
| G: -5717.87902 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11983.34923 HOMO: -7.04503 LUMO: -1.08301 factor:1 | 1 (-1.10451) | -1 | -1 |
| G: -5717.87902 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.18697 HOMO: -6.92530 LUMO: -1.29526 factor:1 | -1 (0.05774) | -1 | -1 |
| G: -5717.87902 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.97077 HOMO: -6.93074 LUMO: -1.25444 factor:1 | 1 (-0.72605) | -1 | -1 |
| G: -5717.87902 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.81890 HOMO: -6.73482 LUMO: -0.62042 factor:1 | 1 (-0.57419) | -1 | -1 |
| G: -5717.87902 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.09617 HOMO: -7.67633 LUMO: 0.59593 factor:1 | -1 (0.14855) | 1 | 1 |
| G: -5717.87902 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.89071 HOMO: -7.39061 LUMO: -0.19320 factor:1 | 1 (-0.64600) | 1 | 1 |
| G: -5717.87902 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11983.27739 HOMO: -7.55388 LUMO: -0.20136 factor:1 | 1 (-1.03267) | 1 | 1 |
| G: -5717.87902 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.06909 HOMO: -7.14027 LUMO: -0.99866 factor:1 | -1 (0.17562) | 1 | 1 |
| G: -5717.87902 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.25048 HOMO: -6.75931 LUMO: -0.73199 factor:1 | 1 (-0.00577) | -1 | -1 |
| G: -5717.87902 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.63795 HOMO: -5.45044 LUMO: -0.18776 factor:1 | 1 (-0.39323) | -1 | -1 |
| G: -5717.87902 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.92542 HOMO: -6.70761 LUMO: -0.84083 factor:1 | -1 (0.31930) | -1 | -1 |
| G: -5717.87902 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.75691 HOMO: -6.05453 LUMO: -1.06669 factor:1 | 1 (-0.51220) | -1 | -1 |
| G: -5717.87902 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.13312 HOMO: -6.86815 LUMO: -0.98233 factor:1 | -1 (0.11159) | -1 | -1 |
| G: -5717.87902 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.18501 HOMO: -6.73210 LUMO: -0.95240 factor:1 | -1 (0.05970) | -1 | -1 |
| G: -5717.87902 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.95246 HOMO: -5.89671 LUMO: -1.05036 factor:1 | 1 (-0.70774) | -1 | -1 |
| G: -5717.87902 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.21522 HOMO: -7.61102 LUMO: 0.33470 factor:1 | -1 (0.02950) | 1 | 1 |
| G: -5717.87902 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.00406 HOMO: -7.51034 LUMO: 0.23674 factor:1 | -1 (0.24066) | 1 | 1 |
| G: -5717.87902 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.20422 HOMO: -7.41510 LUMO: 0.62858 factor:1 | -1 (0.04049) | 1 | 1 |
| G: -5717.87902 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11983.11782 HOMO: -6.76203 LUMO: -1.72792 factor:1 | 1 (-0.87310) | -1 | -1 |
| G: -5717.87902 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11983.11447 HOMO: -6.60420 LUMO: -0.45715 factor:1 | 1 (-0.86976) | -1 | -1 |
| G: -5717.87902 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.71066 HOMO: -6.59060 LUMO: -0.58232 factor:1 | 1 (-0.46594) | -1 | -1 |
| G: -5717.87902 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.82601 HOMO: -7.43687 LUMO: -0.76736 factor:1 | -1 (0.41870) | 1 | 1 |
| G: -5717.87902 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.27710 HOMO: -6.08719 LUMO: -0.48708 factor:1 | 1 (-0.03238) | -1 | -1 |
| G: -5717.87902 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.12118 HOMO: -5.88854 LUMO: -0.05714 factor:1 | -1 (0.12354) | -1 | -1 |
| G: -5717.87902 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.23870 HOMO: -7.34435 LUMO: -0.71838 factor:1 | -1 (0.00601) | 1 | 1 |
| G: -5717.87902 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.29462 HOMO: -7.46408 LUMO: -0.63130 factor:1 | 1 (-0.04991) | 1 | 1 |
| G: -5717.87902 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.91929 HOMO: -7.00965 LUMO: -1.24900 factor:1 | -1 (0.32542) | -1 | -1 |
| G: -5717.87902 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.43465 HOMO: -6.91169 LUMO: -0.88981 factor:1 | 1 (-0.18994) | -1 | -1 |
| G: -5717.87902 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.62336 HOMO: -6.78652 LUMO: -0.82178 factor:1 | 1 (-0.37865) | -1 | -1 |
| G: -5717.87902 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.41106 HOMO: -7.80423 LUMO: 0.87076 factor:1 | 1 (-0.16634) | 1 | 1 |
| G: -5717.87902 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.34564 HOMO: -6.97700 LUMO: -1.00954 factor:1 | 1 (-0.10093) | -1 | -1 |
| G: -5717.87902 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.24931 HOMO: -6.92530 LUMO: -0.88165 factor:1 | 1 (-0.00460) | -1 | -1 |
| G: -5717.87902 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.06273 HOMO: -7.14571 LUMO: -1.04492 factor:1 | -1 (1.18198) | 1 | 1 |
| G: -5717.87902 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.30011 HOMO: -7.49674 LUMO: 0.34558 factor:1 | -1 (1.94461) | 1 | 1 |
| G: -5717.87902 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.00437 HOMO: -6.44094 LUMO: -1.20819 factor:1 | -1 (2.24034) | -1 | -1 |
| G: -5717.87902 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11979.92628 HOMO: -6.47359 LUMO: -1.14016 factor:1 | -1 (2.31844) | -1 | -1 |
| G: -5717.87902 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.38899 HOMO: -6.61237 LUMO: -0.87076 factor:1 | 1 (-0.14427) | -1 | -1 |
| G: -5717.87902 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.32752 HOMO: -6.73754 LUMO: -1.09662 factor:1 | 1 (-0.08280) | -1 | -1 |
| G: -5717.87902 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.34643 HOMO: -6.97700 LUMO: 0.13061 factor:1 | 1 (-0.10172) | -1 | -1 |
| G: -5717.87902 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.23669 HOMO: -6.82734 LUMO: 0.59865 factor:1 | -1 (0.00803) | -1 | -1 |
| G: -5717.87902 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.31808 HOMO: -6.86543 LUMO: -0.91430 factor:1 | 1 (-0.07336) | -1 | -1 |
| G: -5717.87902 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.27424 HOMO: -6.74298 LUMO: 0.28028 factor:1 | 1 (-0.02952) | -1 | -1 |
| G: -5717.87902 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.24341 HOMO: -6.75387 LUMO: 0.19592 factor:1 | -1 (0.00131) | -1 | -1 |
| G: -5717.87902 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.12183 HOMO: -7.05591 LUMO: 0.10612 factor:1 | -1 (0.12289) | -1 | -1 |
| G: -5717.87902 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.18048 HOMO: -6.86543 LUMO: 0.49253 factor:1 | -1 (1.06424) | -1 | -1 |
| G: -5717.87902 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.24627 HOMO: -6.11440 LUMO: -1.12655 factor:1 | 1 (-0.00155) | -1 | -1 |
| G: -5717.87902 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.14206 HOMO: -6.77291 LUMO: -1.02859 factor:1 | -1 (2.10265) | -1 | -1 |
| G: -5717.87902 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11979.89635 HOMO: -6.54978 LUMO: 0.29116 factor:1 | -1 (2.34837) | -1 | -1 |
| G: -5717.87902 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.07017 HOMO: -7.18108 LUMO: 0.00000 factor:1 | -1 (2.17454) | 1 | 1 |
| G: -5717.87902 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11979.93866 HOMO: -6.86271 LUMO: -1.15376 factor:1 | -1 (2.30606) | -1 | -1 |
| G: -5717.87902 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.02765 HOMO: -6.78108 LUMO: -1.22723 factor:1 | -1 (0.21707) | -1 | -1 |
| G: -5717.87902 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.17846 HOMO: -6.40828 LUMO: 0.02449 factor:1 | -1 (1.06625) | -1 | -1 |
| G: -5717.87902 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.88332 HOMO: -6.43821 LUMO: 0.09796 factor:1 | -1 (0.36139) | -1 | -1 |
| G: -5717.87902 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.92929 HOMO: -6.99877 LUMO: 0.40545 factor:1 | -1 (1.31543) | -1 | -1 |
| G: -5717.87902 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.93314 HOMO: -6.68856 LUMO: 0.19320 factor:1 | -1 (0.31157) | -1 | -1 |
| G: -5717.87902 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.13868 HOMO: -7.11034 LUMO: 0.31293 factor:1 | -1 (1.10603) | 1 | 1 |
| G: -5717.87902 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.10633 HOMO: -6.92530 LUMO: -0.85444 factor:1 | -1 (1.13839) | -1 | -1 |
| G: -5717.87902 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.15327 HOMO: -6.60148 LUMO: -0.59865 factor:1 | -1 (1.09145) | -1 | -1 |
| G: -5717.87902 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.93362 HOMO: -6.72938 LUMO: 0.30749 factor:1 | -1 (1.31110) | -1 | -1 |
| G: -5717.87902 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.94083 HOMO: -7.31170 LUMO: 0.06803 factor:1 | -1 (1.30389) | 1 | 1 |
| G: -5717.87902 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.87751 HOMO: -7.09129 LUMO: -0.04626 factor:1 | -1 (1.36721) | 1 | 1 |
| G: -5717.87902 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.62928 HOMO: -6.38379 LUMO: -0.76736 factor:1 | -1 (1.61543) | -1 | -1 |
| G: -5717.87902 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.72455 HOMO: -6.13617 LUMO: -0.63947 factor:1 | -1 (1.52016) | -1 | -1 |
| G: -5717.87902 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.06197 HOMO: -6.92258 LUMO: 0.37007 factor:1 | -1 (1.18274) | -1 | -1 |
| G: -5717.87902 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.94736 HOMO: -6.35930 LUMO: 0.41361 factor:1 | -1 (1.29736) | -1 | -1 |
| G: -5717.87902 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.31001 HOMO: -6.60420 LUMO: 0.26667 factor:1 | -1 (1.93470) | -1 | -1 |
| G: -5717.87902 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.88725 HOMO: -6.04909 LUMO: 1.82588 factor:1 | -1 (1.35747) | -1 | -1 |
| G: -5717.87902 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.62879 HOMO: -6.69672 LUMO: 1.72520 factor:1 | -1 (1.61592) | -1 | -1 |
| G: -5717.87902 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.51587 HOMO: -6.50080 LUMO: 0.29116 factor:1 | -1 (1.72885) | -1 | -1 |
| G: -5717.87902 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.94646 HOMO: -6.60692 LUMO: -0.43266 factor:1 | -1 (1.29826) | -1 | -1 |
| G: -5717.87902 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.67459 HOMO: -6.93890 LUMO: 0.39729 factor:1 | -1 (1.57012) | -1 | -1 |
| G: -5717.87902 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.38153 HOMO: -6.52801 LUMO: -0.47076 factor:1 | 1 (-0.13682) | -1 | -1 |
| G: -5717.87902 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.34766 HOMO: -6.41100 LUMO: 0.30477 factor:1 | 1 (-0.10294) | -1 | -1 |
| G: -5717.87902 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.14534 HOMO: -6.37291 LUMO: -0.80001 factor:1 | -1 (0.09938) | -1 | -1 |
| G: -5717.87902 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.83075 HOMO: -6.51985 LUMO: 1.44765 factor:1 | -1 (0.41397) | -1 | -1 |
| G: -5717.87902 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.91597 HOMO: -6.64774 LUMO: 0.04626 factor:1 | -1 (0.32874) | -1 | -1 |
| G: -5717.87902 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.75777 HOMO: -6.65863 LUMO: 0.29933 factor:1 | -1 (0.48695) | -1 | -1 |
| G: -5717.87902 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.43705 HOMO: -7.09673 LUMO: 0.28300 factor:1 | -1 (0.80766) | 1 | 1 |
| G: -5717.87902 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.64043 HOMO: -6.57155 LUMO: -1.11567 factor:1 | -1 (0.60428) | -1 | -1 |
| G: -5717.87902 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.31644 HOMO: -6.38379 LUMO: -0.60681 factor:1 | 1 (-0.07173) | -1 | -1 |
| G: -5717.87902 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11983.43902 HOMO: -6.60148 LUMO: 0.18232 factor:1 | 1 (-1.19431) | -1 | -1 |
| G: -5717.87902 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.42134 HOMO: -6.96067 LUMO: -0.52246 factor:1 | 1 (-0.17663) | -1 | -1 |
| G: -5717.87902 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11983.36065 HOMO: -6.57427 LUMO: -0.84627 factor:1 | 1 (-1.11594) | -1 | -1 |
| G: -5717.87902 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.71036 HOMO: -6.59332 LUMO: -0.98233 factor:1 | 1 (-0.46564) | -1 | -1 |
| G: -5717.87902 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.06795 HOMO: -6.20692 LUMO: -0.27483 factor:1 | -1 (0.17677) | -1 | -1 |
| G: -5717.87902 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.81270 HOMO: -6.81373 LUMO: 0.74559 factor:1 | 1 (-0.56798) | -1 | -1 |
| G: -5717.87902 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.40431 HOMO: -6.60420 LUMO: 0.54695 factor:1 | 1 (-0.15959) | -1 | -1 |
| G: -5717.87902 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.48466 HOMO: -6.58788 LUMO: -0.31021 factor:1 | 1 (-0.23995) | -1 | -1 |
| G: -5717.87902 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.27701 HOMO: -6.72938 LUMO: 0.64763 factor:1 | 1 (-0.03230) | -1 | -1 |
| G: -5717.87902 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.79275 HOMO: -6.86815 LUMO: 0.32109 factor:1 | 1 (-0.54804) | -1 | -1 |
| G: -5717.87902 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.98422 HOMO: -6.63141 LUMO: 0.18776 factor:1 | -1 (0.26049) | -1 | -1 |
| G: -5717.87902 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.89396 HOMO: -7.18653 LUMO: 0.09524 factor:1 | -1 (0.35075) | 1 | 1 |
| G: -5717.87902 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.29993 HOMO: -6.83550 LUMO: 0.03537 factor:1 | 1 (-0.05521) | -1 | -1 |
| G: -5717.87902 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11983.05619 HOMO: -7.47769 LUMO: 0.40817 factor:1 | 1 (-0.81147) | 1 | 1 |
| G: -5717.87902 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.94277 HOMO: -6.57971 LUMO: -0.63675 factor:1 | 1 (-0.69805) | -1 | -1 |
| G: -5717.87902 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.13288 HOMO: -6.74842 LUMO: -0.16327 factor:1 | -1 (0.11184) | -1 | -1 |
| G: -5717.87902 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.05783 HOMO: -7.07224 LUMO: 0.61770 factor:1 | -1 (0.18689) | 1 | 1 |
| G: -5717.87902 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.40428 HOMO: -6.83006 LUMO: 0.54695 factor:1 | 1 (-0.15957) | -1 | -1 |
| G: -5717.87902 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.52498 HOMO: -6.60148 LUMO: 1.23540 factor:1 | -1 (1.71973) | -1 | -1 |
| G: -5717.87902 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.91215 HOMO: -6.99061 LUMO: 0.41089 factor:1 | -1 (1.33257) | -1 | -1 |
| G: -5717.87902 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.67048 HOMO: -6.63686 LUMO: 0.85172 factor:1 | -1 (1.57423) | -1 | -1 |
| G: -5717.87902 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.80189 HOMO: -6.50624 LUMO: 0.12517 factor:1 | -1 (1.44283) | -1 | -1 |
| G: -5717.87902 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.17753 HOMO: -6.35658 LUMO: 0.36463 factor:1 | -1 (0.06718) | -1 | -1 |
| G: -5717.87902 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.29819 HOMO: -6.34570 LUMO: 0.65035 factor:1 | 1 (-0.05347) | -1 | -1 |
| G: -5717.87902 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.89869 HOMO: -6.63141 LUMO: 1.25717 factor:1 | -1 (0.34602) | -1 | -1 |
| G: -5717.87902 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.65743 HOMO: -6.91441 LUMO: 1.32792 factor:1 | 1 (-0.41272) | -1 | -1 |
| G: -5717.87902 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.54678 HOMO: -7.15387 LUMO: 0.64219 factor:1 | -1 (1.69794) | 1 | 1 |
| G: -5717.87902 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.62392 HOMO: -7.17836 LUMO: 0.60409 factor:1 | -1 (1.62079) | 1 | 1 |
| G: -5717.87902 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.55810 HOMO: -6.92258 LUMO: 0.49525 factor:1 | -1 (1.68662) | -1 | -1 |
| G: -5717.87902 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.47407 HOMO: -6.31032 LUMO: 0.48708 factor:1 | -1 (1.77064) | -1 | -1 |
| G: -5717.87902 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.77650 HOMO: -6.49808 LUMO: 0.31021 factor:1 | -1 (1.46822) | -1 | -1 |
| G: -5717.87902 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.93968 HOMO: -6.48447 LUMO: 0.37552 factor:1 | -1 (1.30503) | -1 | -1 |
| G: -5717.87902 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.66654 HOMO: -6.66135 LUMO: -1.08301 factor:1 | -1 (1.57818) | -1 | -1 |
| G: -5717.87902 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.89535 HOMO: -6.33481 LUMO: -0.51974 factor:1 | -1 (0.34937) | -1 | -1 |
| G: -5717.87902 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.99301 HOMO: -6.76475 LUMO: -0.15238 factor:1 | -1 (0.25171) | -1 | -1 |
| G: -5717.87902 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.71330 HOMO: -6.93346 LUMO: -0.10885 factor:1 | -1 (0.53141) | -1 | -1 |
| G: -5717.87902 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.47012 HOMO: -7.19741 LUMO: 0.73199 factor:1 | -1 (0.77460) | 1 | 1 |
| G: -5717.87902 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.81875 HOMO: -6.82734 LUMO: 0.88437 factor:1 | -1 (0.42597) | -1 | -1 |
| G: -5717.87902 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.62794 HOMO: -7.01237 LUMO: 0.02721 factor:1 | -1 (0.61677) | -1 | -1 |
| G: -5717.87902 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.12749 HOMO: -6.39195 LUMO: 1.46941 factor:1 | -1 (0.11723) | -1 | -1 |
| G: -5717.87902 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.62929 HOMO: -6.53890 LUMO: 1.32792 factor:1 | 1 (-0.38458) | -1 | -1 |
| G: -5717.87902 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.87950 HOMO: -6.82734 LUMO: 1.98099 factor:1 | 1 (-0.63479) | -1 | -1 |
| G: -5717.87902 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.04044 HOMO: -6.74570 LUMO: 1.68983 factor:1 | -1 (0.20428) | -1 | -1 |
| G: -5717.87902 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11983.19973 HOMO: -6.41100 LUMO: 1.39050 factor:1 | 1 (-0.95501) | -1 | -1 |
| G: -5717.87902 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.69615 HOMO: -5.92664 LUMO: 1.65989 factor:1 | 1 (-0.45144) | -1 | -1 |
| G: -5717.87902 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.48330 HOMO: -6.07630 LUMO: 1.54833 factor:1 | 1 (-0.23859) | -1 | -1 |
| G: -5717.87902 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.70192 HOMO: -6.45998 LUMO: 0.68573 factor:1 | 1 (-0.45721) | -1 | -1 |
| G: -5717.87902 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.92218 HOMO: -6.52801 LUMO: 0.41361 factor:1 | -1 (0.32254) | -1 | -1 |
| G: -5717.87902 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.80871 HOMO: -6.77564 LUMO: 0.42178 factor:1 | -1 (0.43601) | -1 | -1 |
| G: -5717.87902 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11983.11733 HOMO: -6.56339 LUMO: 1.65717 factor:1 | 1 (-0.87261) | -1 | -1 |
| G: -5717.87902 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.30499 HOMO: -5.85861 LUMO: 1.90752 factor:1 | 1 (-0.06027) | -1 | -1 |
| G: -5717.87902 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.16795 HOMO: -6.77019 LUMO: -2.48440 factor:1 | -1 (0.07676) | -1 | -1 |
| G: -5717.87902 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.16705 HOMO: -6.53890 LUMO: -1.82588 factor:1 | -1 (0.07766) | -1 | -1 |
| G: -5717.87902 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.82865 HOMO: -6.50352 LUMO: -1.66806 factor:1 | -1 (0.41606) | -1 | -1 |
| G: -5717.87902 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.83575 HOMO: -6.90625 LUMO: 0.43538 factor:1 | -1 (0.40896) | -1 | -1 |
| G: -5717.87902 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.75709 HOMO: -6.85455 LUMO: 0.53062 factor:1 | -1 (0.48763) | -1 | -1 |
| G: -5717.87902 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.66457 HOMO: -6.49536 LUMO: 0.31021 factor:1 | -1 (0.58015) | -1 | -1 |
| G: -5717.87902 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.23963 HOMO: -4.97696 LUMO: -0.09252 factor:1 | -1 (0.00509) | -1 | -1 |
| G: -5717.87902 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.33538 HOMO: -5.31166 LUMO: 0.34286 factor:1 | 1 (-0.09067) | -1 | -1 |
| G: -5717.87902 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.72185 HOMO: -6.42461 LUMO: 0.74287 factor:1 | -1 (0.52287) | -1 | -1 |
| G: -5717.87902 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.58653 HOMO: -6.59604 LUMO: 0.62858 factor:1 | -1 (0.65819) | -1 | -1 |
| G: -5717.87902 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.24578 HOMO: -6.45998 LUMO: -0.61770 factor:1 | -1 (0.99893) | -1 | -1 |
| G: -5717.87902 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.30999 HOMO: -6.75659 LUMO: -0.34014 factor:1 | 1 (-0.06528) | -1 | -1 |
| G: -5717.87902 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.23432 HOMO: -6.63958 LUMO: 0.36191 factor:1 | -1 (0.01039) | -1 | -1 |
| G: -5717.87902 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.04966 HOMO: -5.92936 LUMO: -0.67484 factor:1 | -1 (0.19505) | -1 | -1 |
| G: -5717.87902 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.81448 HOMO: -5.67630 LUMO: 1.80956 factor:1 | -1 (0.43024) | -1 | -1 |
| G: -5717.87902 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.92104 HOMO: -6.50352 LUMO: -0.78369 factor:1 | -1 (0.32368) | -1 | -1 |
| G: -5717.87902 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.11881 HOMO: -6.35930 LUMO: -0.75648 factor:1 | -1 (0.12591) | -1 | -1 |
| G: -5717.87902 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.81647 HOMO: -6.74298 LUMO: 0.48980 factor:1 | -1 (1.42824) | -1 | -1 |
| G: -5717.87902 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.82593 HOMO: -6.85183 LUMO: 0.15510 factor:1 | -1 (0.41878) | -1 | -1 |
| G: -5717.87902 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.87268 HOMO: -6.90897 LUMO: 0.26123 factor:1 | -1 (0.37203) | -1 | -1 |
| G: -5717.87902 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.08328 HOMO: -6.85999 LUMO: 0.47892 factor:1 | -1 (1.16144) | -1 | -1 |
| G: -5717.87902 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.87487 HOMO: -6.69944 LUMO: 0.57416 factor:1 | -1 (1.36985) | -1 | -1 |
| G: -5717.87902 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.93530 HOMO: -6.74026 LUMO: 0.69933 factor:1 | -1 (1.30941) | -1 | -1 |
| G: -5717.87902 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.06711 HOMO: -6.52801 LUMO: 0.75376 factor:1 | -1 (1.17760) | -1 | -1 |
| G: -5717.87902 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.11185 HOMO: -7.05863 LUMO: 0.44627 factor:1 | -1 (1.13286) | -1 | -1 |
| G: -5717.87902 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.13852 HOMO: -6.96339 LUMO: 0.48164 factor:1 | -1 (1.10620) | -1 | -1 |
| G: -5717.87902 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.89476 HOMO: -6.95795 LUMO: 0.44355 factor:1 | -1 (1.34996) | -1 | -1 |
| G: -5717.87902 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.53935 HOMO: -6.36746 LUMO: 0.58777 factor:1 | -1 (1.70536) | -1 | -1 |
| G: -5717.87902 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.18584 HOMO: -6.69400 LUMO: 0.40545 factor:1 | -1 (1.05888) | -1 | -1 |
| G: -5717.87902 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.04333 HOMO: -6.30760 LUMO: -0.66668 factor:1 | -1 (1.20138) | -1 | -1 |
| G: -5717.87902 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.58759 HOMO: -6.53617 LUMO: -0.64491 factor:1 | -1 (0.65713) | -1 | -1 |
| G: -5717.87902 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.08218 HOMO: -6.80829 LUMO: 0.17415 factor:1 | -1 (0.16253) | -1 | -1 |
| G: -5717.87902 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.95033 HOMO: -6.80285 LUMO: 0.73471 factor:1 | 1 (-0.70562) | -1 | -1 |
| G: -5717.87902 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.91867 HOMO: -6.43821 LUMO: 0.21769 factor:1 | -1 (0.32605) | -1 | -1 |
| G: -5717.87902 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.91339 HOMO: -6.98788 LUMO: 0.10885 factor:1 | -1 (0.33133) | -1 | -1 |
| G: -5717.87902 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.04755 HOMO: -7.15115 LUMO: 0.40817 factor:1 | -1 (1.19716) | 1 | 1 |
| G: -5717.87902 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.82866 HOMO: -6.00011 LUMO: -0.98505 factor:1 | -1 (1.41605) | -1 | -1 |
| G: -5717.87902 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.84061 HOMO: -6.16882 LUMO: -0.77825 factor:1 | -1 (1.40411) | -1 | -1 |
| G: -5717.87902 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.79642 HOMO: -6.30760 LUMO: 0.34831 factor:1 | -1 (1.44830) | -1 | -1 |
| G: -5717.87902 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.98058 HOMO: -6.64502 LUMO: 0.63403 factor:1 | -1 (1.26413) | -1 | -1 |
| G: -5717.87902 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.83726 HOMO: -6.93618 LUMO: 0.96600 factor:1 | -1 (1.40745) | -1 | -1 |
| G: -5717.87902 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.93446 HOMO: -6.45182 LUMO: 0.16327 factor:1 | -1 (1.31026) | -1 | -1 |
| G: -5717.87902 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.79791 HOMO: -6.99605 LUMO: 0.20953 factor:1 | -1 (1.44680) | -1 | -1 |
| G: -5717.87902 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.09565 HOMO: -6.72665 LUMO: 0.32654 factor:1 | -1 (0.14906) | -1 | -1 |
| G: -5717.87902 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.24893 HOMO: -6.38379 LUMO: 0.45443 factor:1 | 1 (-0.00422) | -1 | -1 |
| G: -5717.87902 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.82480 HOMO: -6.65318 LUMO: 0.04354 factor:1 | -1 (1.41992) | -1 | -1 |
| G: -5717.87902 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.85176 HOMO: -6.94707 LUMO: -1.68438 factor:1 | -1 (1.39295) | -1 | -1 |
| G: -5717.87902 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.80735 HOMO: -6.71849 LUMO: 0.15783 factor:1 | -1 (0.43737) | -1 | -1 |
| G: -5717.87902 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.86041 HOMO: -6.97156 LUMO: 0.43266 factor:1 | -1 (0.38431) | -1 | -1 |
| G: -5717.87902 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.38572 HOMO: -6.91441 LUMO: -0.54695 factor:1 | 1 (-0.14101) | -1 | -1 |
| G: -5717.87902 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11983.43532 HOMO: -6.74842 LUMO: -0.76192 factor:1 | 1 (-1.19061) | -1 | -1 |
| G: -5717.87902 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11983.51614 HOMO: -6.70489 LUMO: 0.19048 factor:1 | 1 (-1.27142) | -1 | -1 |
| G: -5717.87902 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.69196 HOMO: -7.25728 LUMO: 0.33470 factor:1 | 1 (-0.44725) | 1 | -1 |
| G: -5717.87902 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11983.50896 HOMO: -6.96339 LUMO: 0.55511 factor:1 | 1 (-1.26424) | -1 | -1 |
| G: -5717.87902 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11983.23997 HOMO: -6.77564 LUMO: 0.72382 factor:1 | 1 (-0.99526) | -1 | -1 |
| G: -5717.87902 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.42613 HOMO: -6.75387 LUMO: 0.39729 factor:1 | 1 (-0.18142) | -1 | -1 |
| G: -5717.87902 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.43997 HOMO: -7.00149 LUMO: 0.06531 factor:1 | -1 (0.80475) | -1 | -1 |
| G: -5717.87902 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.39789 HOMO: -7.09945 LUMO: 0.33470 factor:1 | 1 (-0.15317) | 1 | 1 |
| G: -5717.87902 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.42885 HOMO: -7.20830 LUMO: 0.59593 factor:1 | 1 (-0.18414) | 1 | 1 |
| G: -5717.87902 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.46886 HOMO: -6.40556 LUMO: 0.56600 factor:1 | -1 (0.77585) | -1 | -1 |
| G: -5717.87902 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.55646 HOMO: -6.77291 LUMO: 0.73471 factor:1 | -1 (0.68826) | -1 | -1 |
| G: -5717.87902 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.28031 HOMO: -6.65046 LUMO: 0.09796 factor:1 | 1 (-0.03559) | -1 | -1 |
| G: -5717.87902 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.24093 HOMO: -6.95795 LUMO: 0.22313 factor:1 | -1 (0.00378) | -1 | -1 |
| G: -5717.87902 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.13765 HOMO: -6.85727 LUMO: 0.04626 factor:1 | -1 (1.10707) | -1 | -1 |
| G: -5717.87902 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.71926 HOMO: -7.27360 LUMO: 0.42178 factor:1 | -1 (0.52545) | 1 | 1 |
| G: -5717.87902 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.36701 HOMO: -6.78924 LUMO: -0.13334 factor:1 | -1 (0.87770) | -1 | -1 |
| G: -5717.87902 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.45394 HOMO: -6.63141 LUMO: 0.38368 factor:1 | 1 (-0.20923) | -1 | -1 |
| G: -5717.87902 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.23873 HOMO: -6.92258 LUMO: 0.39184 factor:1 | -1 (0.00599) | -1 | -1 |
| G: -5717.87902 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.41330 HOMO: -6.19331 LUMO: -0.46804 factor:1 | -1 (0.83142) | -1 | -1 |
| G: -5717.87902 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.51681 HOMO: -7.26544 LUMO: -0.05442 factor:1 | -1 (0.72790) | 1 | 1 |
| G: -5717.87902 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.90544 HOMO: -7.09401 LUMO: 0.30749 factor:1 | -1 (0.33927) | 1 | 1 |
| G: -5717.87902 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.12256 HOMO: -6.14705 LUMO: -0.88709 factor:1 | -1 (0.12215) | -1 | -1 |
| G: -5717.87902 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.30967 HOMO: -6.53617 LUMO: -0.28572 factor:1 | 1 (-0.06495) | -1 | -1 |
| G: -5717.87902 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.13261 HOMO: -6.37291 LUMO: -0.67212 factor:1 | -1 (1.11210) | -1 | -1 |
| G: -5717.87902 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.75584 HOMO: -6.65591 LUMO: 0.03810 factor:1 | -1 (1.48887) | -1 | -1 |
| G: -5717.87902 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.07593 HOMO: -7.11034 LUMO: 0.75103 factor:1 | -1 (1.16878) | 1 | 1 |
| G: -5717.87902 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.35063 HOMO: -6.85183 LUMO: -0.05987 factor:1 | -1 (0.89408) | -1 | -1 |
| G: -5717.87902 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.26316 HOMO: -6.70761 LUMO: -0.05442 factor:1 | 1 (-0.01845) | -1 | -1 |
| G: -5717.87902 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.12738 HOMO: -6.23413 LUMO: 0.06259 factor:1 | -1 (0.11734) | -1 | -1 |
| G: -5717.87902 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.51572 HOMO: -6.55794 LUMO: 0.74015 factor:1 | -1 (0.72899) | -1 | -1 |
| G: -5717.87902 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.32255 HOMO: -7.27905 LUMO: 0.26939 factor:1 | -1 (0.92217) | 1 | 1 |
| G: -5717.87902 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.13239 HOMO: -6.34842 LUMO: -0.86804 factor:1 | -1 (0.11233) | -1 | -1 |
| G: -5717.87902 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.61596 HOMO: -6.27222 LUMO: 1.46125 factor:1 | 1 (-0.37124) | -1 | -1 |
| G: -5717.87902 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.70013 HOMO: -6.65046 LUMO: 2.04902 factor:1 | -1 (0.54458) | -1 | -1 |
| G: -5717.87902 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.06901 HOMO: -7.11850 LUMO: -1.14016 factor:1 | -1 (0.17570) | 1 | -1 |
| G: -5717.87902 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11983.29916 HOMO: -6.88720 LUMO: -1.20274 factor:1 | 1 (-1.05444) | -1 | -1 |
| G: -5717.87902 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11983.61767 HOMO: -6.69400 LUMO: -0.31565 factor:1 | 1 (-1.37295) | -1 | -1 |
| G: -5717.87902 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11983.76131 HOMO: -6.95523 LUMO: -1.55377 factor:1 | 1 (-1.51660) | -1 | -1 |
| G: -5717.87902 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11983.19496 HOMO: -6.41372 LUMO: -0.83539 factor:1 | 1 (-0.95025) | -1 | -1 |
| G: -5717.87902 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11983.57807 HOMO: -6.13889 LUMO: -0.90070 factor:1 | 1 (-1.33336) | -1 | -1 |
| G: -5717.87902 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.78505 HOMO: -6.44366 LUMO: -0.55511 factor:1 | 1 (-0.54034) | -1 | -1 |
| G: -5717.87902 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.20216 HOMO: -6.10079 LUMO: -0.71022 factor:1 | -1 (0.04256) | -1 | -1 |
| G: -5717.87902 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.64023 HOMO: -6.90353 LUMO: -0.64763 factor:1 | 1 (-0.39552) | -1 | -1 |
| G: -5717.87902 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.43518 HOMO: -6.65046 LUMO: -0.82450 factor:1 | -1 (0.80954) | -1 | -1 |
| G: -5717.87902 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.60669 HOMO: -6.81645 LUMO: -0.85444 factor:1 | -1 (0.63803) | -1 | -1 |
| G: -5717.87902 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.04060 HOMO: -6.20692 LUMO: 1.30887 factor:1 | -1 (0.20411) | -1 | -1 |
| G: -5717.87902 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.76773 HOMO: -5.96201 LUMO: 1.33880 factor:1 | -1 (0.47699) | -1 | -1 |
| G: -5717.87902 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.63653 HOMO: -6.52529 LUMO: 1.58914 factor:1 | 1 (-0.39182) | -1 | -1 |
| G: -5717.87902 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.84411 HOMO: -6.58516 LUMO: 1.97555 factor:1 | -1 (0.40061) | -1 | -1 |
| G: -5717.87902 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.91277 HOMO: -6.84366 LUMO: 0.15783 factor:1 | -1 (1.33194) | -1 | -1 |
| G: -5717.87902 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.84066 HOMO: -6.45726 LUMO: 0.42994 factor:1 | -1 (1.40405) | -1 | -1 |
| G: -5717.87902 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.70384 HOMO: -6.75387 LUMO: 0.14422 factor:1 | -1 (1.54087) | -1 | -1 |
| G: -5717.87902 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.92022 HOMO: -6.69944 LUMO: 1.79051 factor:1 | -1 (0.32450) | -1 | -1 |
| G: -5717.87902 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.27278 HOMO: -6.59876 LUMO: 1.90208 factor:1 | -1 (0.97194) | -1 | -1 |
| G: -5717.87902 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.23365 HOMO: -7.05863 LUMO: 1.20819 factor:1 | -1 (1.01107) | -1 | -1 |
| G: -5717.87902 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.04918 HOMO: -6.54978 LUMO: 2.01636 factor:1 | -1 (1.19553) | -1 | -1 |
| G: -5717.87902 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.05527 HOMO: -5.52119 LUMO: 1.95106 factor:1 | -1 (0.18945) | -1 | -1 |
| G: -5717.87902 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.95442 HOMO: -6.53617 LUMO: 1.60275 factor:1 | 1 (-0.70970) | -1 | -1 |
| G: -5717.87902 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.25574 HOMO: -6.11440 LUMO: 1.89119 factor:1 | 1 (-0.01102) | -1 | -1 |
| G: -5717.87902 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11983.32465 HOMO: -7.31986 LUMO: 0.48708 factor:1 | 1 (-1.07994) | 1 | 1 |
| G: -5717.87902 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.22526 HOMO: -6.76475 LUMO: -0.75648 factor:1 | -1 (0.01946) | -1 | -1 |
| G: -5717.87902 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11983.11137 HOMO: -6.76747 LUMO: -1.06941 factor:1 | 1 (-0.86666) | -1 | -1 |
| G: -5717.87902 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11983.18432 HOMO: -6.87087 LUMO: 0.72927 factor:1 | 1 (-0.93961) | -1 | -1 |
| G: -5717.87902 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.41816 HOMO: -7.00965 LUMO: 0.02177 factor:1 | 1 (-0.17345) | -1 | -1 |
| G: -5717.87902 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.44475 HOMO: -6.54706 LUMO: -0.03265 factor:1 | 1 (-0.20003) | -1 | -1 |
| G: -5717.87902 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.06760 HOMO: -6.62325 LUMO: -0.63675 factor:1 | -1 (1.17711) | -1 | -1 |
| G: -5717.87902 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.97875 HOMO: -7.03414 LUMO: -1.24084 factor:1 | -1 (0.26596) | -1 | -1 |
| G: -5717.87902 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.93067 HOMO: -7.04503 LUMO: -0.10068 factor:1 | -1 (0.31405) | -1 | -1 |
| G: -5717.87902 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.87943 HOMO: -6.67223 LUMO: 0.03537 factor:1 | -1 (0.36529) | -1 | -1 |
| G: -5717.87902 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.06319 HOMO: -6.82734 LUMO: 0.58777 factor:1 | -1 (0.18153) | -1 | -1 |
| G: -5717.87902 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.97415 HOMO: -6.84366 LUMO: 0.46531 factor:1 | -1 (0.27056) | -1 | -1 |
| G: -5717.87902 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.96030 HOMO: -7.03959 LUMO: -1.15104 factor:1 | -1 (0.28441) | -1 | -1 |
| G: -5717.87902 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.93973 HOMO: -6.91169 LUMO: -0.41361 factor:1 | -1 (0.30499) | -1 | -1 |
| G: -5717.87902 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.94251 HOMO: -7.10217 LUMO: -0.44627 factor:1 | -1 (0.30221) | 1 | 1 |
| G: -5717.87902 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.87385 HOMO: -6.88176 LUMO: -0.19592 factor:1 | -1 (0.37086) | -1 | -1 |
| G: -5717.87902 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.15794 HOMO: -7.21374 LUMO: -0.46531 factor:1 | -1 (0.08678) | 1 | 1 |
| G: -5717.87902 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.90748 HOMO: -6.54978 LUMO: 0.16871 factor:1 | -1 (0.33723) | -1 | -1 |
| G: -5717.87902 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.70090 HOMO: -6.71305 LUMO: -0.13061 factor:1 | -1 (0.54382) | -1 | -1 |
| G: -5717.87902 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.74830 HOMO: -6.74842 LUMO: -0.36191 factor:1 | -1 (0.49642) | -1 | -1 |
| G: -5717.87902 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.43980 HOMO: -6.74570 LUMO: -0.09796 factor:1 | -1 (0.80491) | -1 | -1 |
| G: -5717.87902 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.70606 HOMO: -6.93890 LUMO: -0.27211 factor:1 | 1 (-0.46134) | -1 | -1 |
| G: -5717.87902 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.97647 HOMO: -6.88720 LUMO: -0.18776 factor:1 | -1 (0.26825) | -1 | -1 |
| G: -5717.87902 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.85107 HOMO: -6.74842 LUMO: 0.02993 factor:1 | -1 (0.39364) | -1 | -1 |
| G: -5717.87902 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.99660 HOMO: -6.70216 LUMO: 0.01361 factor:1 | -1 (0.24811) | -1 | -1 |
| G: -5717.87902 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.98106 HOMO: -6.90625 LUMO: 0.00544 factor:1 | -1 (0.26365) | -1 | -1 |
| G: -5717.87902 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.70753 HOMO: -6.18243 LUMO: 0.25851 factor:1 | -1 (0.53718) | -1 | -1 |
| G: -5717.87902 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.82833 HOMO: -6.32937 LUMO: -0.20953 factor:1 | -1 (0.41639) | -1 | -1 |
| G: -5717.87902 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.69235 HOMO: -6.78108 LUMO: 0.00544 factor:1 | -1 (0.55236) | -1 | -1 |
| G: -5717.87902 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.50174 HOMO: -5.97562 LUMO: 0.28572 factor:1 | -1 (0.74298) | -1 | -1 |
| G: -5717.87902 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.95377 HOMO: -5.97290 LUMO: -0.18504 factor:1 | -1 (0.29094) | -1 | -1 |
| G: -5717.87902 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.07840 HOMO: -6.12800 LUMO: 0.42178 factor:1 | -1 (0.16632) | -1 | -1 |
| G: -5717.87902 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.10896 HOMO: -6.24229 LUMO: -0.00816 factor:1 | -1 (0.13576) | -1 | -1 |
| G: -5717.87902 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11983.23543 HOMO: -6.61781 LUMO: 0.12789 factor:1 | 1 (-0.99071) | -1 | -1 |
| G: -5717.87902 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11983.17415 HOMO: -6.70489 LUMO: 0.14694 factor:1 | 1 (-0.92943) | -1 | -1 |
| G: -5717.87902 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.35669 HOMO: -6.86543 LUMO: -0.21225 factor:1 | 1 (-0.11197) | -1 | -1 |
| G: -5717.87902 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.91734 HOMO: -6.90081 LUMO: -0.20136 factor:1 | -1 (1.32737) | -1 | -1 |
| G: -5717.87902 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.65244 HOMO: -7.12938 LUMO: -0.25851 factor:1 | -1 (1.59227) | 1 | 1 |
| G: -5717.87902 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.48327 HOMO: -6.93074 LUMO: -0.26667 factor:1 | -1 (1.76145) | -1 | -1 |
| G: -5717.87902 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.80262 HOMO: -7.00421 LUMO: -0.31021 factor:1 | -1 (1.44209) | -1 | -1 |
| G: -5717.87902 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.73405 HOMO: -7.10761 LUMO: -0.17415 factor:1 | -1 (1.51067) | 1 | 1 |
| G: -5717.87902 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.62318 HOMO: -8.21240 LUMO: 0.05987 factor:1 | -1 (0.62154) | 1 | 1 |
| G: -5717.87902 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.99320 HOMO: -7.14843 LUMO: -0.46531 factor:1 | -1 (0.25151) | 1 | -1 |
| G: -5717.87902 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.75717 HOMO: -6.80829 LUMO: -0.29933 factor:1 | -1 (0.48755) | -1 | -1 |
| G: -5717.87902 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.52677 HOMO: -6.84094 LUMO: -0.53606 factor:1 | -1 (0.71795) | -1 | -1 |
| G: -5717.87902 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.68903 HOMO: -6.81917 LUMO: -0.26667 factor:1 | -1 (0.55568) | -1 | -1 |
| G: -5717.87902 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.87611 HOMO: -6.85727 LUMO: -1.20002 factor:1 | -1 (0.36861) | -1 | -1 |
| G: -5717.87902 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.94435 HOMO: -6.39468 LUMO: -1.06941 factor:1 | 1 (-0.69963) | -1 | -1 |
| G: -5717.87902 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.99198 HOMO: -6.00827 LUMO: -1.94017 factor:1 | -1 (0.25274) | -1 | -1 |
| G: -5717.87902 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.73542 HOMO: -6.80829 LUMO: 0.18504 factor:1 | 1 (-0.49070) | -1 | -1 |
| G: -5717.87902 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.80482 HOMO: -6.54434 LUMO: -0.95784 factor:1 | -1 (0.43990) | -1 | -1 |
| G: -5717.87902 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.50067 HOMO: -6.45454 LUMO: -0.07347 factor:1 | -1 (0.74404) | -1 | -1 |
| G: -5717.87902 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.67616 HOMO: -5.33887 LUMO: 1.11839 factor:1 | -1 (0.56855) | -1 | -1 |
| G: -5717.87902 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.43022 HOMO: -5.75249 LUMO: 0.70477 factor:1 | -1 (0.81449) | -1 | -1 |
| G: -5717.87902 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.89235 HOMO: -5.64092 LUMO: 0.87076 factor:1 | -1 (0.35236) | -1 | -1 |
| G: -5717.87902 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.83535 HOMO: -5.14295 LUMO: 1.06124 factor:1 | -1 (0.40937) | -1 | -1 |
| G: -5717.87902 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.33887 HOMO: -5.05043 LUMO: 1.21091 factor:1 | 1 (-0.09415) | -1 | -1 |
| G: -5717.87902 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.62927 HOMO: -5.05588 LUMO: 1.02859 factor:1 | -1 (0.61544) | -1 | -1 |
| G: -5717.87902 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.22188 HOMO: -5.76337 LUMO: 0.79457 factor:1 | -1 (0.02283) | -1 | -1 |
| G: -5717.87902 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.49597 HOMO: -5.01506 LUMO: 1.00138 factor:1 | -1 (0.74875) | -1 | -1 |
| G: -5717.87902 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.23476 HOMO: -4.84363 LUMO: 1.53744 factor:1 | -1 (1.00995) | -1 | -1 |
| G: -5717.87902 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.33569 HOMO: -5.17833 LUMO: 1.45309 factor:1 | -1 (0.90902) | -1 | -1 |
| G: -5717.87902 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.96885 HOMO: -5.13751 LUMO: 0.51157 factor:1 | -1 (1.27586) | -1 | -1 |
| G: -5717.87902 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11979.94786 HOMO: -5.56473 LUMO: 0.32109 factor:1 | -1 (2.29686) | -1 | -1 |
| G: -5717.87902 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11979.84859 HOMO: -4.69941 LUMO: 1.14016 factor:1 | -1 (2.39613) | -1 | -1 |
| G: -5717.87902 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.07970 HOMO: -4.49260 LUMO: 1.86398 factor:1 | -1 (2.16502) | -1 | -1 |
| G: -5717.87902 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11979.94073 HOMO: -4.32117 LUMO: 1.68438 factor:1 | -1 (2.30399) | -1 | -1 |
| G: -5717.87902 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.12681 HOMO: -4.44906 LUMO: 1.37690 factor:1 | -1 (0.11791) | -1 | -1 |
| G: -5717.87902 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.34235 HOMO: -4.62049 LUMO: 1.34968 factor:1 | 1 (-0.09763) | -1 | -1 |
| G: -5717.87902 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.93399 HOMO: -4.59600 LUMO: 1.58370 factor:1 | -1 (0.31073) | -1 | -1 |
| G: -5717.87902 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.27051 HOMO: -4.98785 LUMO: 1.46669 factor:1 | 1 (-0.02580) | -1 | -1 |
| G: -5717.87902 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.60753 HOMO: -5.06676 LUMO: 1.27349 factor:1 | -1 (0.63718) | -1 | -1 |
| G: -5717.87902 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.48206 HOMO: -5.09125 LUMO: 1.13471 factor:1 | -1 (0.76265) | -1 | -1 |
| G: -5717.87902 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.40026 HOMO: -4.84635 LUMO: 1.33608 factor:1 | 1 (-0.15554) | -1 | -1 |
| G: -5717.87902 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.42635 HOMO: -4.94431 LUMO: 1.18370 factor:1 | 1 (-0.18164) | -1 | -1 |
| G: -5717.87902 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.76890 HOMO: -4.92526 LUMO: 1.39867 factor:1 | -1 (0.47582) | -1 | -1 |
| G: -5717.87902 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.19391 HOMO: -5.71983 LUMO: 0.60137 factor:1 | -1 (0.05080) | -1 | -1 |
| G: -5717.87902 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.23840 HOMO: -5.10486 LUMO: 1.05580 factor:1 | -1 (0.00631) | -1 | -1 |
| G: -5717.87902 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.58457 HOMO: -5.20282 LUMO: 1.01226 factor:1 | -1 (0.66015) | -1 | -1 |
| G: -5717.87902 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.04667 HOMO: -4.98513 LUMO: 1.53744 factor:1 | -1 (0.19804) | -1 | -1 |
| G: -5717.87902 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.37286 HOMO: -5.67085 LUMO: 0.17687 factor:1 | -1 (0.87185) | -1 | -1 |
| G: -5717.87902 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.22900 HOMO: -5.87222 LUMO: 0.12517 factor:1 | -1 (1.01572) | -1 | -1 |
| G: -5717.87902 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.02003 HOMO: -5.20826 LUMO: 0.91702 factor:1 | -1 (0.22468) | -1 | -1 |
| G: -5717.87902 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.89954 HOMO: -5.94569 LUMO: 0.63130 factor:1 | -1 (0.34518) | -1 | -1 |
| G: -5717.87902 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.47822 HOMO: -5.35792 LUMO: 0.91430 factor:1 | -1 (0.76649) | -1 | -1 |
| G: -5717.87902 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.41609 HOMO: -5.36336 LUMO: 1.44220 factor:1 | 1 (-0.17138) | -1 | -1 |
| G: -5717.87902 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.34564 HOMO: -5.83412 LUMO: 0.71294 factor:1 | 1 (-0.10093) | -1 | -1 |
| G: -5717.87902 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.28912 HOMO: -4.97696 LUMO: 1.72792 factor:1 | 1 (-0.04441) | -1 | -1 |
| G: -5717.87902 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.32300 HOMO: -5.55929 LUMO: 0.23130 factor:1 | 1 (-0.07829) | -1 | -1 |
| G: -5717.87902 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.15323 HOMO: -5.71167 LUMO: 0.47348 factor:1 | -1 (0.09148) | -1 | -1 |
| G: -5717.87902 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.20358 HOMO: -7.31986 LUMO: -2.54699 factor:1 | -1 (1.04113) | -1 | -1 |
| G: -5717.87902 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.21916 HOMO: -5.34704 LUMO: 1.19730 factor:1 | -1 (0.02555) | -1 | -1 |
| G: -5717.87902 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.43664 HOMO: -5.45860 LUMO: 0.80818 factor:1 | 1 (-0.19192) | -1 | -1 |
| G: -5717.87902 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11979.88786 HOMO: -5.12663 LUMO: 1.20274 factor:1 | -1 (2.35686) | -1 | -1 |
| G: -5717.87902 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11979.87643 HOMO: -5.37153 LUMO: 1.05580 factor:1 | -1 (2.36829) | -1 | -1 |
| G: -5717.87902 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11979.94127 HOMO: -5.47221 LUMO: 0.97961 factor:1 | -1 (2.30344) | -1 | -1 |
| G: -5717.87902 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.06097 HOMO: -5.06948 LUMO: 1.12111 factor:1 | -1 (2.18374) | -1 | -1 |
| G: -5717.87902 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.33507 HOMO: -5.19737 LUMO: 1.25444 factor:1 | -1 (0.90965) | -1 | -1 |
| G: -5717.87902 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.92420 HOMO: -5.27901 LUMO: 1.00682 factor:1 | -1 (1.32051) | -1 | -1 |
| G: -5717.87902 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.66986 HOMO: -5.38513 LUMO: 0.49253 factor:1 | -1 (1.57486) | -1 | -1 |
| G: -5717.87902 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.04347 HOMO: -5.12390 LUMO: 1.22995 factor:1 | -1 (1.20125) | -1 | -1 |
| G: -5717.87902 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.70596 HOMO: -5.31438 LUMO: 0.70205 factor:1 | -1 (0.53876) | -1 | -1 |
| G: -5717.87902 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.85615 HOMO: -5.17561 LUMO: 1.04492 factor:1 | -1 (1.38857) | -1 | -1 |
| G: -5717.87902 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.87484 HOMO: -4.94431 LUMO: 1.52656 factor:1 | -1 (1.36988) | -1 | -1 |
| G: -5717.87902 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.86171 HOMO: -5.13751 LUMO: 0.93879 factor:1 | -1 (0.38300) | -1 | -1 |
| G: -5717.87902 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.05041 HOMO: -5.49942 LUMO: 0.97689 factor:1 | -1 (1.19431) | -1 | -1 |
| G: -5717.87902 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.94417 HOMO: -5.79058 LUMO: 0.53879 factor:1 | -1 (1.30054) | -1 | -1 |
| G: -5717.87902 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.94894 HOMO: -5.36881 LUMO: 1.56465 factor:1 | -1 (1.29578) | -1 | -1 |
| G: -5717.87902 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11979.41781 HOMO: -4.67492 LUMO: 1.32792 factor:1 | -1 (2.82691) | -1 | -1 |
| G: -5717.87902 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.08514 HOMO: -4.60145 LUMO: 1.19458 factor:1 | -1 (2.15958) | -1 | -1 |
| G: -5717.87902 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.31053 HOMO: -4.49260 LUMO: 1.60547 factor:1 | -1 (1.93419) | -1 | -1 |
| G: -5717.87902 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11979.92854 HOMO: -4.65043 LUMO: 1.34696 factor:1 | -1 (2.31618) | -1 | -1 |
| G: -5717.87902 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.03148 HOMO: -4.77560 LUMO: 1.35241 factor:1 | -1 (2.21324) | -1 | -1 |
| G: -5717.87902 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.13034 HOMO: -4.94431 LUMO: 1.17825 factor:1 | -1 (2.11438) | -1 | -1 |
| G: -5717.87902 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.29292 HOMO: -4.87084 LUMO: 1.41771 factor:1 | -1 (1.95179) | -1 | -1 |
| G: -5717.87902 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.71666 HOMO: -5.34432 LUMO: 1.16737 factor:1 | -1 (1.52806) | -1 | -1 |
| G: -5717.87902 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.94420 HOMO: -4.94975 LUMO: 1.67622 factor:1 | -1 (1.30051) | -1 | -1 |
| G: -5717.87902 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11979.89025 HOMO: -4.81369 LUMO: 1.14288 factor:1 | -1 (2.35447) | -1 | -1 |
| G: -5717.87902 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11979.88315 HOMO: -5.22459 LUMO: 0.29660 factor:1 | -1 (2.36157) | -1 | -1 |
| G: -5717.87902 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11979.87594 HOMO: -5.21642 LUMO: 0.37824 factor:1 | -1 (2.36878) | -1 | -1 |
| G: -5717.87902 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.09684 HOMO: -5.00417 LUMO: 1.01226 factor:1 | -1 (2.14788) | -1 | -1 |
| G: -5717.87902 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.10400 HOMO: -5.46677 LUMO: 0.10612 factor:1 | -1 (2.14072) | -1 | -1 |
| G: -5717.87902 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.34817 HOMO: -5.51303 LUMO: 0.54151 factor:1 | 1 (-0.10346) | -1 | -1 |
| G: -5717.87902 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.97429 HOMO: -5.63004 LUMO: 0.17960 factor:1 | -1 (0.27043) | -1 | -1 |
| G: -5717.87902 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.41294 HOMO: -4.79193 LUMO: 1.12111 factor:1 | 1 (-0.16822) | -1 | -1 |
| G: -5717.87902 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.31010 HOMO: -5.43411 LUMO: 0.45987 factor:1 | 1 (-0.06539) | -1 | -1 |
| G: -5717.87902 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.04490 HOMO: -7.06135 LUMO: -2.13881 factor:1 | -1 (0.19981) | 1 | 1 |
| G: -5717.87902 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.27663 HOMO: -5.33071 LUMO: 1.14016 factor:1 | 1 (-0.03192) | -1 | -1 |
| G: -5717.87902 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.05464 HOMO: -7.12394 LUMO: -0.03810 factor:1 | -1 (0.19007) | 1 | 1 |
| G: -5717.87902 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.76247 HOMO: -7.20558 LUMO: -2.50889 factor:1 | -1 (0.48224) | 1 | 1 |
| G: -5717.87902 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.17280 HOMO: -7.26816 LUMO: -2.11432 factor:1 | -1 (0.07192) | 1 | 1 |
| G: -5717.87902 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.83427 HOMO: -7.89674 LUMO: 0.31021 factor:1 | -1 (1.41045) | 1 | 1 |
| G: -5717.87902 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.46149 HOMO: -7.26544 LUMO: 0.22858 factor:1 | -1 (0.78323) | 1 | 1 |
| G: -5717.87902 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.77696 HOMO: -7.12666 LUMO: -0.02449 factor:1 | -1 (1.46775) | 1 | 1 |
| G: -5717.87902 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.21531 HOMO: -7.68722 LUMO: 0.71838 factor:1 | -1 (1.02941) | 1 | 1 |
| G: -5717.87902 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.56349 HOMO: -6.86271 LUMO: -0.96056 factor:1 | -1 (1.68123) | -1 | -1 |
| G: -5717.87902 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.38219 HOMO: -7.07496 LUMO: -1.11839 factor:1 | 1 (-0.13747) | 1 | 1 |
| G: -5717.87902 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.33944 HOMO: -7.06952 LUMO: -2.08439 factor:1 | 1 (-0.09472) | 1 | 1 |
| G: -5717.87902 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.74770 HOMO: -6.60965 LUMO: -2.11977 factor:1 | -1 (0.49702) | -1 | -1 |
| G: -5717.87902 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.26629 HOMO: -6.87360 LUMO: -1.85854 factor:1 | 1 (-0.02158) | -1 | -1 |
| G: -5717.87902 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.26284 HOMO: -7.67089 LUMO: -0.24762 factor:1 | 1 (-0.01812) | 1 | 1 |
| G: -5717.87902 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.67806 HOMO: -6.45726 LUMO: -1.86398 factor:1 | -1 (0.56665) | -1 | -1 |
| G: -5717.87902 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.26758 HOMO: -6.91713 LUMO: 0.33198 factor:1 | -1 (0.97713) | -1 | -1 |
| G: -5717.87902 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.04477 HOMO: -6.83278 LUMO: 0.26667 factor:1 | -1 (0.19995) | -1 | -1 |
| G: -5717.87902 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.44639 HOMO: -6.89264 LUMO: -1.00682 factor:1 | -1 (0.79833) | -1 | -1 |
| G: -5717.87902 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.99081 HOMO: -6.57427 LUMO: 0.22041 factor:1 | -1 (1.25390) | -1 | -1 |
| G: -5717.87902 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11979.69686 HOMO: -7.52123 LUMO: -0.01905 factor:1 | -1 (2.54786) | 1 | 1 |
| G: -5717.87902 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11979.91626 HOMO: -7.37429 LUMO: -0.08980 factor:1 | -1 (2.32845) | 1 | 1 |
| G: -5717.87902 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11979.98176 HOMO: -7.28449 LUMO: -0.26395 factor:1 | -1 (2.26295) | 1 | 1 |
| G: -5717.87902 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11979.04270 HOMO: -6.79740 LUMO: -0.60954 factor:1 | -1 (3.20202) | -1 | -1 |
| G: -5717.87902 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11979.29195 HOMO: -7.12666 LUMO: -0.60681 factor:1 | -1 (2.95276) | 1 | 1 |
| G: -5717.87902 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11979.25568 HOMO: -6.96611 LUMO: -0.30477 factor:1 | -1 (2.98903) | -1 | -1 |
| G: -5717.87902 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11979.05821 HOMO: -7.08040 LUMO: -0.31293 factor:1 | -1 (3.18651) | 1 | 1 |
| G: -5717.87902 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.12024 HOMO: -6.78924 LUMO: -0.73743 factor:1 | -1 (2.12447) | -1 | -1 |
| G: -5717.87902 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11979.74597 HOMO: -7.57293 LUMO: -1.11295 factor:1 | -1 (2.49874) | 1 | 1 |
| G: -5717.87902 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11979.93409 HOMO: -7.15932 LUMO: -0.23130 factor:1 | -1 (2.31063) | 1 | 1 |
| G: -5717.87902 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11979.99978 HOMO: -7.48585 LUMO: -0.10068 factor:1 | -1 (2.24494) | 1 | 1 |
| G: -5717.87902 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.14574 HOMO: -7.17020 LUMO: -0.26123 factor:1 | -1 (2.09898) | 1 | 1 |
| G: -5717.87902 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11979.76540 HOMO: -7.43143 LUMO: -0.16055 factor:1 | -1 (2.47931) | 1 | 1 |
| G: -5717.87902 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.65981 HOMO: -7.14843 LUMO: -0.10612 factor:1 | -1 (1.58490) | 1 | 1 |
| G: -5717.87902 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.09228 HOMO: -6.95523 LUMO: -0.22585 factor:1 | -1 (0.15244) | -1 | -1 |
| G: -5717.87902 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.81630 HOMO: -7.06680 LUMO: -0.51974 factor:1 | -1 (0.42842) | 1 | 1 |
| G: -5717.87902 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.30039 HOMO: -6.80829 LUMO: -0.64763 factor:1 | 1 (-0.05567) | -1 | -1 |
| G: -5717.87902 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.74011 HOMO: -7.13210 LUMO: -0.48164 factor:1 | -1 (0.50461) | 1 | 1 |
| G: -5717.87902 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.37166 HOMO: -7.16204 LUMO: -0.45715 factor:1 | -1 (0.87305) | 1 | 1 |
| G: -5717.87902 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.37171 HOMO: -7.15115 LUMO: -0.43266 factor:1 | 1 (-0.12700) | 1 | 1 |
| G: -5717.87902 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.81241 HOMO: -7.15932 LUMO: -2.52794 factor:1 | -1 (0.43231) | -1 | -1 |
| G: -5717.87902 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.49686 HOMO: -7.21102 LUMO: -2.65311 factor:1 | 1 (-0.25214) | -1 | -1 |
| G: -5717.87902 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.25590 HOMO: -6.57427 LUMO: -2.78645 factor:1 | 1 (-0.01118) | -1 | -1 |
| G: -5717.87902 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.12237 HOMO: -6.40828 LUMO: -3.23815 factor:1 | -1 (0.12234) | -1 | -1 |
| G: -5717.87902 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.12550 HOMO: -7.71987 LUMO: -0.20953 factor:1 | -1 (0.11921) | 1 | 1 |
| G: -5717.87902 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.47028 HOMO: -7.47769 LUMO: -0.43810 factor:1 | -1 (0.77444) | 1 | 1 |
| G: -5717.87902 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.35552 HOMO: -6.68040 LUMO: -2.22589 factor:1 | 1 (-0.11080) | -1 | -1 |
| G: -5717.87902 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.51980 HOMO: -6.92802 LUMO: -1.99187 factor:1 | -1 (0.72491) | -1 | -1 |
| G: -5717.87902 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.31470 HOMO: -7.73620 LUMO: 0.01633 factor:1 | 1 (-0.06999) | 1 | 1 |
| G: -5717.87902 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.13960 HOMO: -7.28721 LUMO: -0.18504 factor:1 | -1 (0.10512) | 1 | 1 |
| G: -5717.87902 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.25952 HOMO: -7.49674 LUMO: -0.19864 factor:1 | 1 (-0.01480) | 1 | 1 |
| G: -5717.87902 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.99701 HOMO: -7.10489 LUMO: -2.56331 factor:1 | -1 (0.24771) | -1 | -1 |
| G: -5717.87902 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.28908 HOMO: -7.36612 LUMO: 0.16055 factor:1 | -1 (0.95564) | 1 | 1 |
| G: -5717.87902 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.56536 HOMO: -7.67633 LUMO: 0.33198 factor:1 | -1 (0.67936) | 1 | 1 |
| G: -5717.87902 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.29365 HOMO: -7.07768 LUMO: -0.27483 factor:1 | -1 (0.95107) | 1 | 1 |
| G: -5717.87902 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.83423 HOMO: -7.32531 LUMO: 0.05442 factor:1 | -1 (0.41048) | 1 | 1 |
| G: -5717.87902 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.66106 HOMO: -6.79740 LUMO: -1.21635 factor:1 | -1 (0.58366) | -1 | -1 |
| G: -5717.87902 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.83026 HOMO: -7.14027 LUMO: 0.12517 factor:1 | -1 (0.41446) | 1 | -1 |
| G: -5717.87902 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.95764 HOMO: -7.17292 LUMO: 0.16871 factor:1 | -1 (1.28707) | 1 | -1 |
| G: -5717.87902 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.08619 HOMO: -7.08312 LUMO: -1.38778 factor:1 | -1 (1.15852) | 1 | 1 |
| G: -5717.87902 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.31485 HOMO: -6.75387 LUMO: -1.88031 factor:1 | -1 (0.92987) | -1 | -1 |
| G: -5717.87902 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.11980 HOMO: -7.07768 LUMO: -1.25717 factor:1 | -1 (1.12492) | 1 | 1 |
| G: -5717.87902 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11979.81297 HOMO: -6.46543 LUMO: -1.14016 factor:1 | -1 (2.43175) | -1 | -1 |
| G: -5717.87902 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.05017 HOMO: -7.37973 LUMO: -0.45987 factor:1 | -1 (2.19454) | 1 | 1 |
| G: -5717.87902 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11979.90116 HOMO: -7.46408 LUMO: 0.03265 factor:1 | -1 (2.34355) | 1 | 1 |
| G: -5717.87902 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.21953 HOMO: -7.96477 LUMO: -0.19864 factor:1 | -1 (1.02519) | 1 | 1 |
| G: -5717.87902 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.36513 HOMO: -6.93890 LUMO: -1.11839 factor:1 | -1 (0.87958) | -1 | -1 |
| G: -5717.87902 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.85317 HOMO: -7.06408 LUMO: -1.08846 factor:1 | -1 (0.39154) | 1 | 1 |
| G: -5717.87902 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.37674 HOMO: -7.14027 LUMO: -0.33470 factor:1 | 1 (-0.13203) | 1 | 1 |
| G: -5717.87902 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.36627 HOMO: -7.38245 LUMO: 0.10885 factor:1 | 1 (-0.12155) | 1 | 1 |
| G: -5717.87902 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.08398 HOMO: -7.59470 LUMO: -1.21363 factor:1 | -1 (0.16074) | 1 | 1 |
| G: -5717.87902 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.15870 HOMO: -7.23279 LUMO: -1.23812 factor:1 | -1 (0.08602) | 1 | 1 |
| G: -5717.87902 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.10743 HOMO: -6.90897 LUMO: 0.23402 factor:1 | -1 (0.13728) | -1 | -1 |
| G: -5717.87902 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.41782 HOMO: -7.36340 LUMO: -0.17143 factor:1 | -1 (0.82690) | 1 | 1 |
| G: -5717.87902 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.14426 HOMO: -6.61781 LUMO: -0.01361 factor:1 | -1 (1.10046) | -1 | -1 |
| G: -5717.87902 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.29794 HOMO: -6.80013 LUMO: 0.38368 factor:1 | 1 (-0.05323) | -1 | -1 |
| G: -5717.87902 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.87619 HOMO: -6.72121 LUMO: -0.95512 factor:1 | -1 (0.36852) | -1 | -1 |
| G: -5717.87902 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11979.77876 HOMO: -6.24773 LUMO: -0.69933 factor:1 | -1 (2.46595) | -1 | -1 |
| G: -5717.87902 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11979.84769 HOMO: -6.56883 LUMO: 0.14694 factor:1 | -1 (2.39702) | -1 | -1 |
| G: -5717.87902 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.04160 HOMO: -6.51441 LUMO: -1.27621 factor:1 | -1 (2.20312) | -1 | -1 |
| G: -5717.87902 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.12076 HOMO: -6.91986 LUMO: -1.16737 factor:1 | -1 (2.12396) | -1 | -1 |
| G: -5717.87902 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11979.88391 HOMO: -6.17971 LUMO: -0.65307 factor:1 | -1 (2.36081) | -1 | -1 |
| G: -5717.87902 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.80533 HOMO: -7.22462 LUMO: 0.04354 factor:1 | -1 (0.43938) | 1 | 1 |
| G: -5717.87902 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.82126 HOMO: -7.16204 LUMO: -0.23674 factor:1 | -1 (1.42345) | 1 | 1 |
| G: -5717.87902 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.60364 HOMO: -6.81645 LUMO: -0.19320 factor:1 | -1 (0.64107) | -1 | -1 |
| G: -5717.87902 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.74945 HOMO: -6.69400 LUMO: 0.04082 factor:1 | -1 (1.49527) | -1 | -1 |
| G: -5717.87902 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.55045 HOMO: -6.63141 LUMO: -0.22858 factor:1 | -1 (1.69426) | -1 | -1 |
| G: -5717.87902 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.80515 HOMO: -6.92258 LUMO: -1.11295 factor:1 | -1 (1.43956) | -1 | -1 |
| G: -5717.87902 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.82163 HOMO: -6.60148 LUMO: -1.13744 factor:1 | -1 (0.42308) | -1 | -1 |
| G: -5717.87902 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.95158 HOMO: -6.78108 LUMO: -0.82450 factor:1 | -1 (1.29314) | -1 | -1 |
| G: -5717.87902 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.74790 HOMO: -7.05591 LUMO: -0.97145 factor:1 | -1 (1.49682) | -1 | -1 |
| G: -5717.87902 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.05743 HOMO: -6.65318 LUMO: -1.26261 factor:1 | -1 (1.18729) | -1 | -1 |
| G: -5717.87902 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.85451 HOMO: -6.98244 LUMO: -0.98233 factor:1 | -1 (1.39020) | -1 | -1 |
| G: -5717.87902 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11979.97284 HOMO: -7.11850 LUMO: -0.99594 factor:1 | -1 (2.27188) | 1 | 1 |
| G: -5717.87902 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11979.97926 HOMO: -6.64230 LUMO: -0.93879 factor:1 | -1 (2.26546) | -1 | -1 |
| G: -5717.87902 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.77906 HOMO: -6.62053 LUMO: -1.22451 factor:1 | -1 (1.46566) | -1 | -1 |
| G: -5717.87902 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11979.80622 HOMO: -7.02598 LUMO: -0.85172 factor:1 | -1 (2.43849) | -1 | -1 |
| G: -5717.87902 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.02818 HOMO: -7.06680 LUMO: -0.89253 factor:1 | -1 (2.21653) | 1 | 1 |
| G: -5717.87902 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.07531 HOMO: -7.17292 LUMO: 0.00272 factor:1 | -1 (2.16940) | 1 | 1 |
| G: -5717.87902 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11979.84742 HOMO: -7.03142 LUMO: -0.35103 factor:1 | -1 (2.39730) | -1 | -1 |
| G: -5717.87902 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.39598 HOMO: -6.96884 LUMO: -0.09796 factor:1 | 1 (-0.15127) | -1 | -1 |
| G: -5717.87902 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.59433 HOMO: -6.56339 LUMO: -0.99322 factor:1 | 1 (-0.34961) | -1 | -1 |
| G: -5717.87902 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.16463 HOMO: -7.08857 LUMO: -0.17687 factor:1 | -1 (0.08008) | 1 | 1 |
| G: -5717.87902 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.07688 HOMO: -7.05863 LUMO: -0.22041 factor:1 | -1 (0.16784) | -1 | -1 |
| G: -5717.87902 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.29737 HOMO: -7.15115 LUMO: -0.17960 factor:1 | 1 (-0.05265) | 1 | 1 |
| G: -5717.87902 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.82128 HOMO: -6.67495 LUMO: -0.96600 factor:1 | -1 (0.42344) | -1 | -1 |
| G: -5717.87902 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11983.48784 HOMO: -6.74026 LUMO: -1.79867 factor:1 | 1 (-1.24312) | -1 | -1 |
| G: -5717.87902 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.59914 HOMO: -6.73482 LUMO: -1.78235 factor:1 | 1 (-0.35443) | -1 | -1 |
| G: -5717.87902 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11983.40172 HOMO: -6.09807 LUMO: 0.16871 factor:1 | 1 (-1.15700) | -1 | -1 |
| G: -5717.87902 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.39936 HOMO: -6.72393 LUMO: 0.27211 factor:1 | 1 (-0.15464) | -1 | -1 |
| G: -5717.87902 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.57844 HOMO: -6.40556 LUMO: -0.04354 factor:1 | 1 (-0.33372) | -1 | -1 |
| G: -5717.87902 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.91665 HOMO: -6.56883 LUMO: 0.22041 factor:1 | 1 (-0.67193) | -1 | -1 |
| G: -5717.87902 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.19620 HOMO: -7.22462 LUMO: 0.15783 factor:1 | -1 (0.04852) | 1 | 1 |
| G: -5717.87902 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.90275 HOMO: -6.83550 LUMO: 0.19320 factor:1 | -1 (0.34197) | -1 | -1 |
| G: -5717.87902 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.11451 HOMO: -7.26816 LUMO: -0.07619 factor:1 | -1 (0.13021) | 1 | -1 |
| G: -5717.87902 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.83313 HOMO: -7.13483 LUMO: 0.33198 factor:1 | 1 (-0.58842) | 1 | 1 |
| G: -5717.87902 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.76674 HOMO: -6.58243 LUMO: -0.26395 factor:1 | 1 (-0.52202) | -1 | -1 |
| G: -5717.87902 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.04716 HOMO: -7.38517 LUMO: 0.17143 factor:1 | -1 (0.19755) | 1 | 1 |
| G: -5717.87902 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.32991 HOMO: -6.80013 LUMO: 0.25851 factor:1 | 1 (-0.08520) | -1 | -1 |
| G: -5717.87902 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.98965 HOMO: -6.96611 LUMO: 0.11429 factor:1 | 1 (-0.74494) | -1 | -1 |
| G: -5717.87902 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.91452 HOMO: -6.51713 LUMO: -1.14560 factor:1 | 1 (-0.66981) | -1 | -1 |
| G: -5717.87902 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.20480 HOMO: -7.15387 LUMO: -0.35647 factor:1 | -1 (0.03992) | 1 | 1 |
| G: -5717.87902 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.82531 HOMO: -5.26540 LUMO: 1.26805 factor:1 | -1 (0.41941) | -1 | -1 |
| G: -5717.87902 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.34956 HOMO: -6.76475 LUMO: -0.16327 factor:1 | 1 (-0.10485) | -1 | -1 |
| G: -5717.87902 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.09532 HOMO: -6.55250 LUMO: -0.71838 factor:1 | -1 (0.14939) | -1 | -1 |
| G: -5717.87902 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11979.88592 HOMO: -6.76203 LUMO: -1.08301 factor:1 | -1 (2.35879) | -1 | -1 |
| G: -5717.87902 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.09602 HOMO: -7.14027 LUMO: -0.01633 factor:1 | -1 (2.14869) | 1 | 1 |
| G: -5717.87902 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.32856 HOMO: -6.94979 LUMO: -0.93879 factor:1 | -1 (0.91615) | -1 | -1 |
| G: -5717.87902 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.43958 HOMO: -6.74842 LUMO: 0.31293 factor:1 | -1 (0.80513) | -1 | -1 |
| G: -5717.87902 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.15416 HOMO: -6.43821 LUMO: 0.05987 factor:1 | -1 (1.09055) | -1 | -1 |
| G: -5717.87902 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.97988 HOMO: -6.60420 LUMO: 0.22585 factor:1 | -1 (1.26484) | -1 | -1 |
| G: -5717.87902 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.69989 HOMO: -6.43821 LUMO: 0.05987 factor:1 | -1 (0.54483) | -1 | -1 |
| G: -5717.87902 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.85641 HOMO: -6.34570 LUMO: 1.43948 factor:1 | -1 (0.38831) | -1 | -1 |
| G: -5717.87902 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.00801 HOMO: -6.03004 LUMO: 1.21363 factor:1 | -1 (1.23670) | -1 | -1 |
| G: -5717.87902 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.89966 HOMO: -6.68040 LUMO: -0.92247 factor:1 | -1 (1.34506) | -1 | -1 |
| G: -5717.87902 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.61938 HOMO: -6.92530 LUMO: -0.31293 factor:1 | -1 (1.62534) | -1 | -1 |
| G: -5717.87902 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.84072 HOMO: -6.94979 LUMO: -0.19864 factor:1 | -1 (1.40400) | -1 | -1 |
| G: -5717.87902 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.18703 HOMO: -6.80829 LUMO: -0.30477 factor:1 | -1 (0.05769) | -1 | -1 |
| G: -5717.87902 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.85184 HOMO: -7.22734 LUMO: -1.02859 factor:1 | -1 (0.39288) | 1 | 1 |
| G: -5717.87902 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.79309 HOMO: -6.93890 LUMO: -0.72382 factor:1 | -1 (0.45163) | -1 | -1 |
| G: -5717.87902 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.70988 HOMO: -7.27088 LUMO: -0.78097 factor:1 | -1 (0.53484) | 1 | 1 |
| G: -5717.87902 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.02520 HOMO: -7.29809 LUMO: -0.97145 factor:1 | -1 (0.21951) | 1 | 1 |
| G: -5717.87902 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.86433 HOMO: -7.18925 LUMO: -0.94696 factor:1 | -1 (0.38039) | 1 | 1 |
| G: -5717.87902 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.30485 HOMO: -7.33891 LUMO: -0.96873 factor:1 | 1 (-0.06014) | 1 | 1 |
| G: -5717.87902 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11983.32193 HOMO: -7.36068 LUMO: -0.28028 factor:1 | 1 (-1.07722) | 1 | 1 |
| G: -5717.87902 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.71308 HOMO: -7.10761 LUMO: -1.14832 factor:1 | 1 (-0.46836) | 1 | 1 |
| G: -5717.87902 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.86132 HOMO: -6.94707 LUMO: -0.65307 factor:1 | 1 (-0.61661) | -1 | -1 |
| G: -5717.87902 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.15908 HOMO: -6.91713 LUMO: -1.81228 factor:1 | -1 (0.08563) | -1 | -1 |
| G: -5717.87902 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.88705 HOMO: -6.78652 LUMO: -2.01636 factor:1 | -1 (0.35767) | -1 | -1 |
| G: -5717.87902 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.69844 HOMO: -6.52801 LUMO: -1.17553 factor:1 | 1 (-0.45372) | -1 | -1 |
| G: -5717.87902 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.94068 HOMO: -7.54844 LUMO: -1.18642 factor:1 | -1 (0.30403) | 1 | -1 |
| G: -5717.87902 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.92539 HOMO: -7.52939 LUMO: -1.23812 factor:1 | -1 (0.31933) | 1 | -1 |
| G: -5717.87902 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.97012 HOMO: -7.94572 LUMO: -0.81634 factor:1 | 1 (-0.72540) | 1 | 1 |
| G: -5717.87902 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.24278 HOMO: -7.55932 LUMO: -0.86260 factor:1 | -1 (0.00193) | 1 | 1 |
| G: -5717.87902 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.97368 HOMO: -7.72259 LUMO: -1.39050 factor:1 | 1 (-0.72897) | 1 | -1 |
| G: -5717.87902 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.72792 HOMO: -7.11850 LUMO: -1.01498 factor:1 | -1 (0.51680) | 1 | -1 |
| G: -5717.87902 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.97192 HOMO: -7.09673 LUMO: -1.00954 factor:1 | -1 (0.27279) | 1 | -1 |
| G: -5717.87902 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.81101 HOMO: -6.06270 LUMO: 0.16327 factor:1 | 1 (-0.56630) | -1 | -1 |
| G: -5717.87902 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.97627 HOMO: -5.71167 LUMO: 0.70477 factor:1 | -1 (0.26844) | -1 | -1 |
| G: -5717.87902 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.74797 HOMO: -5.38241 LUMO: 0.86260 factor:1 | -1 (0.49674) | -1 | -1 |
| G: -5717.87902 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.60985 HOMO: -5.67357 LUMO: 1.27621 factor:1 | -1 (0.63487) | -1 | -1 |
| G: -5717.87902 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.53406 HOMO: -7.56204 LUMO: -0.68573 factor:1 | -1 (0.71065) | 1 | 1 |
| G: -5717.87902 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.07345 HOMO: -5.57833 LUMO: 1.13199 factor:1 | -1 (0.17127) | -1 | -1 |
| G: -5717.87902 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.22994 HOMO: -7.58653 LUMO: -0.66124 factor:1 | -1 (0.01478) | 1 | 1 |
| G: -5717.87902 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.98874 HOMO: -7.91851 LUMO: -1.10206 factor:1 | -1 (0.25598) | 1 | -1 |
| G: -5717.87902 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.14565 HOMO: -6.48992 LUMO: -1.00138 factor:1 | -1 (1.09907) | -1 | -1 |
| G: -5717.87902 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.98023 HOMO: -7.09673 LUMO: -0.45171 factor:1 | -1 (1.26449) | 1 | 1 |
| G: -5717.87902 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11983.01872 HOMO: -6.63686 LUMO: 0.09252 factor:1 | 1 (-0.77400) | -1 | -1 |
| G: -5717.87902 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.25799 HOMO: -6.84366 LUMO: -0.14422 factor:1 | 1 (-0.01328) | -1 | -1 |
| G: -5717.87902 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.90853 HOMO: -6.93074 LUMO: 0.04354 factor:1 | -1 (1.33619) | -1 | -1 |
| G: -5717.87902 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.97588 HOMO: -6.90353 LUMO: -0.19864 factor:1 | -1 (1.26884) | -1 | -1 |
| G: -5717.87902 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.85986 HOMO: -6.59876 LUMO: -0.10068 factor:1 | -1 (0.38485) | -1 | -1 |
| G: -5717.87902 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.98838 HOMO: -6.74570 LUMO: -0.44627 factor:1 | -1 (0.25633) | -1 | -1 |
| G: -5717.87902 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11983.51666 HOMO: -6.60148 LUMO: -0.61770 factor:1 | 1 (-1.27194) | -1 | -1 |
| G: -5717.87902 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11983.50969 HOMO: -6.55794 LUMO: -1.06941 factor:1 | 1 (-1.26498) | -1 | -1 |
| G: -5717.87902 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.17258 HOMO: -7.12666 LUMO: -0.11973 factor:1 | -1 (0.07214) | 1 | 1 |
| G: -5717.87902 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.16273 HOMO: -7.21646 LUMO: -0.50069 factor:1 | -1 (0.08199) | 1 | 1 |
| G: -5717.87902 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.16428 HOMO: -7.27632 LUMO: -1.00682 factor:1 | -1 (0.08044) | 1 | -1 |
| G: -5717.87902 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.23139 HOMO: -6.74298 LUMO: 0.04354 factor:1 | -1 (1.01332) | -1 | -1 |
| G: -5717.87902 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.36679 HOMO: -6.37291 LUMO: 0.14150 factor:1 | -1 (0.87792) | -1 | -1 |
| G: -5717.87902 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.22146 HOMO: -5.61371 LUMO: 1.28438 factor:1 | -1 (1.02326) | -1 | -1 |
| G: -5717.87902 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.39406 HOMO: -5.52119 LUMO: 0.99866 factor:1 | -1 (0.85066) | -1 | -1 |
| G: -5717.87902 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.41776 HOMO: -6.51985 LUMO: -0.10885 factor:1 | -1 (0.82695) | -1 | -1 |
| G: -5717.87902 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.57662 HOMO: -5.61371 LUMO: 0.77280 factor:1 | -1 (0.66809) | -1 | -1 |
| G: -5717.87902 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.25767 HOMO: -5.58922 LUMO: 0.24490 factor:1 | 1 (-0.01295) | -1 | -1 |
| G: -5717.87902 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11983.44746 HOMO: -6.32665 LUMO: -0.57144 factor:1 | 1 (-1.20274) | -1 | -1 |
| G: -5717.87902 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11983.03406 HOMO: -6.29127 LUMO: -0.93607 factor:1 | 1 (-0.78935) | -1 | -1 |
| G: -5717.87902 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11983.16117 HOMO: -5.49670 LUMO: 0.27211 factor:1 | 1 (-0.91645) | -1 | -1 |
| G: -5717.87902 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.14041 HOMO: -5.68990 LUMO: 0.24218 factor:1 | -1 (0.10430) | -1 | -1 |
| G: -5717.87902 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.79733 HOMO: -5.68174 LUMO: 0.69933 factor:1 | -1 (0.44738) | -1 | -1 |
| G: -5717.87902 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.98618 HOMO: -5.28173 LUMO: 1.00954 factor:1 | -1 (0.25854) | -1 | -1 |
| G: -5717.87902 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.96272 HOMO: -5.94025 LUMO: 0.73471 factor:1 | -1 (0.28199) | -1 | -1 |
| G: -5717.87902 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.76585 HOMO: -5.65725 LUMO: 1.28710 factor:1 | -1 (0.47887) | -1 | -1 |
| G: -5717.87902 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.97045 HOMO: -5.41507 LUMO: 0.87076 factor:1 | -1 (0.27426) | -1 | -1 |
| G: -5717.87902 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.01600 HOMO: -5.96474 LUMO: 0.29660 factor:1 | -1 (0.22871) | -1 | -1 |
| G: -5717.87902 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.80667 HOMO: -7.00421 LUMO: 0.08708 factor:1 | -1 (0.43805) | -1 | -1 |
| G: -5717.87902 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.99938 HOMO: -5.40418 LUMO: 0.90070 factor:1 | -1 (0.24534) | -1 | -1 |
| G: -5717.87902 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11983.04783 HOMO: -7.00421 LUMO: -0.30477 factor:1 | 1 (-0.80312) | -1 | -1 |
| G: -5717.87902 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.82914 HOMO: -5.85861 LUMO: 0.74015 factor:1 | -1 (0.41557) | -1 | -1 |
| G: -5717.87902 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.84985 HOMO: -5.71439 LUMO: 0.26395 factor:1 | -1 (0.39486) | -1 | -1 |
| G: -5717.87902 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.82781 HOMO: -7.13755 LUMO: -0.78369 factor:1 | -1 (0.41691) | 1 | -1 |
| G: -5717.87902 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.85630 HOMO: -7.31442 LUMO: -0.98233 factor:1 | -1 (0.38842) | 1 | -1 |
| G: -5717.87902 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.54563 HOMO: -7.25728 LUMO: -1.00410 factor:1 | -1 (0.69909) | 1 | -1 |
| G: -5717.87902 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.66261 HOMO: -7.48585 LUMO: -0.83811 factor:1 | -1 (0.58211) | 1 | -1 |
| G: -5717.87902 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.74539 HOMO: -7.24911 LUMO: -0.77280 factor:1 | -1 (0.49933) | 1 | -1 |
| G: -5717.87902 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.44394 HOMO: -7.55116 LUMO: -1.19730 factor:1 | -1 (0.80078) | 1 | -1 |
| G: -5717.87902 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.94528 HOMO: -5.76881 LUMO: 0.28028 factor:1 | -1 (0.29943) | -1 | -1 |
| G: -5717.87902 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.04194 HOMO: -5.77153 LUMO: -0.26939 factor:1 | -1 (1.20277) | -1 | -1 |
| G: -5717.87902 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.01250 HOMO: -5.82868 LUMO: 0.36735 factor:1 | -1 (1.23221) | -1 | -1 |
| G: -5717.87902 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.12399 HOMO: -5.83140 LUMO: -0.17960 factor:1 | -1 (1.12073) | -1 | -1 |
| G: -5717.87902 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11979.17334 HOMO: -6.28855 LUMO: 0.01088 factor:1 | -1 (3.07138) | -1 | -1 |
| G: -5717.87902 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.98324 HOMO: -6.31576 LUMO: 0.25307 factor:1 | -1 (0.26147) | -1 | -1 |
| G: -5717.87902 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.03013 HOMO: -7.06408 LUMO: -2.76196 factor:1 | -1 (0.21459) | -1 | -1 |
| G: -5717.87902 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.20131 HOMO: -5.95657 LUMO: 0.37552 factor:1 | -1 (0.04340) | -1 | -1 |
| G: -5717.87902 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.58005 HOMO: -6.61781 LUMO: 0.02721 factor:1 | -1 (0.66467) | -1 | -1 |
| G: -5717.87902 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.26208 HOMO: -6.26678 LUMO: -0.66668 factor:1 | 1 (-0.01736) | -1 | -1 |
| G: -5717.87902 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.50399 HOMO: -6.00011 LUMO: -0.13334 factor:1 | -1 (0.74072) | -1 | -1 |
| G: -5717.87902 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.08224 HOMO: -5.60555 LUMO: 0.67484 factor:1 | -1 (0.16248) | -1 | -1 |
| G: -5717.87902 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.00407 HOMO: -5.79875 LUMO: 0.99049 factor:1 | -1 (1.24065) | -1 | -1 |
| G: -5717.87902 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.71992 HOMO: -5.97834 LUMO: 0.48436 factor:1 | -1 (0.52480) | -1 | -1 |
| G: -5717.87902 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.29503 HOMO: -5.82868 LUMO: 0.91974 factor:1 | 1 (-0.05031) | -1 | -1 |
| G: -5717.87902 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.16967 HOMO: -5.86677 LUMO: 0.99594 factor:1 | -1 (1.07504) | -1 | -1 |
| G: -5717.87902 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.23955 HOMO: -5.70079 LUMO: 0.48980 factor:1 | -1 (1.00516) | -1 | -1 |
| G: -5717.87902 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.99598 HOMO: -7.39605 LUMO: -1.02315 factor:1 | -1 (1.24873) | 1 | -1 |
| G: -5717.87902 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.18159 HOMO: -7.22734 LUMO: -1.12927 factor:1 | -1 (1.06312) | 1 | -1 |
| G: -5717.87902 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.87590 HOMO: -7.58926 LUMO: -0.65035 factor:1 | -1 (1.36881) | 1 | 1 |
| G: -5717.87902 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.55056 HOMO: -7.43959 LUMO: -0.75648 factor:1 | -1 (1.69415) | 1 | 1 |
| G: -5717.87902 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.38981 HOMO: -7.55388 LUMO: -1.15104 factor:1 | -1 (0.85490) | 1 | -1 |
| G: -5717.87902 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.07960 HOMO: -6.74570 LUMO: -2.85447 factor:1 | -1 (1.16511) | -1 | -1 |
| G: -5717.87902 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.81103 HOMO: -7.35524 LUMO: -1.25444 factor:1 | -1 (1.43369) | 1 | 1 |
| G: -5717.87902 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11979.86881 HOMO: -6.81645 LUMO: -1.20819 factor:1 | -1 (2.37591) | -1 | -1 |
| G: -5717.87902 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11979.87071 HOMO: -6.99605 LUMO: -1.62996 factor:1 | -1 (2.37400) | -1 | -1 |
| G: -5717.87902 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.22817 HOMO: -6.88992 LUMO: -0.47620 factor:1 | -1 (0.01654) | -1 | -1 |
| G: -5717.87902 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.89301 HOMO: -7.22190 LUMO: -0.01905 factor:1 | -1 (0.35171) | 1 | 1 |
| G: -5717.87902 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.83970 HOMO: -6.77836 LUMO: -0.82995 factor:1 | -1 (0.40501) | -1 | -1 |
| G: -5717.87902 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.03889 HOMO: -6.48447 LUMO: -0.95512 factor:1 | -1 (0.20583) | -1 | -1 |
| G: -5717.87902 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.10194 HOMO: -7.81239 LUMO: 1.22179 factor:1 | -1 (0.14278) | 1 | 1 |
| G: -5717.87902 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.11206 HOMO: -7.36612 LUMO: 0.19320 factor:1 | -1 (0.13266) | 1 | 1 |
| G: -5717.87902 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.45403 HOMO: -7.24095 LUMO: 0.33470 factor:1 | -1 (0.79068) | 1 | 1 |
| G: -5717.87902 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.12479 HOMO: -7.15932 LUMO: -2.24222 factor:1 | -1 (0.11992) | -1 | -1 |
| G: -5717.87902 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.46160 HOMO: -6.88992 LUMO: -2.69937 factor:1 | -1 (0.78312) | -1 | -1 |
| G: -5717.87902 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.27468 HOMO: -6.97428 LUMO: -0.98233 factor:1 | -1 (0.97003) | -1 | -1 |
| G: -5717.87902 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.03679 HOMO: -7.17564 LUMO: -0.93879 factor:1 | -1 (0.20792) | 1 | 1 |
| G: -5717.87902 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.37207 HOMO: -6.81645 LUMO: -1.14288 factor:1 | -1 (0.87264) | -1 | -1 |
| G: -5717.87902 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.15014 HOMO: -6.83006 LUMO: -0.63403 factor:1 | -1 (1.09458) | -1 | -1 |
| G: -5717.87902 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.05894 HOMO: -7.17292 LUMO: -1.07213 factor:1 | -1 (0.18577) | 1 | 1 |
| G: -5717.87902 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.24344 HOMO: -7.53755 LUMO: 0.15510 factor:1 | -1 (0.00128) | 1 | 1 |
| G: -5717.87902 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.57880 HOMO: -6.50080 LUMO: -0.51702 factor:1 | -1 (0.66592) | -1 | -1 |
| G: -5717.87902 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.35806 HOMO: -6.72665 LUMO: -0.80001 factor:1 | -1 (0.88666) | -1 | -1 |
| G: -5717.87902 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.21478 HOMO: -6.72665 LUMO: 1.68711 factor:1 | -1 (0.02993) | -1 | -1 |
| G: -5717.87902 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.88566 HOMO: -7.11850 LUMO: -0.75103 factor:1 | -1 (0.35905) | 1 | 1 |
| G: -5717.87902 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.78158 HOMO: -6.87087 LUMO: -0.85988 factor:1 | -1 (0.46314) | -1 | -1 |
| G: -5717.87902 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.96996 HOMO: -7.08857 LUMO: -0.89798 factor:1 | -1 (0.27475) | 1 | 1 |
| G: -5717.87902 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.21631 HOMO: -6.71305 LUMO: -0.85444 factor:1 | -1 (1.02840) | -1 | -1 |
| G: -5717.87902 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.40078 HOMO: -6.59332 LUMO: -0.60137 factor:1 | -1 (0.84393) | -1 | -1 |
| G: -5717.87902 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.03566 HOMO: -7.28993 LUMO: 0.03265 factor:1 | -1 (1.20906) | 1 | 1 |
| G: -5717.87902 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.48575 HOMO: -7.32258 LUMO: 0.13878 factor:1 | 1 (-0.24104) | 1 | 1 |
| G: -5717.87902 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.97004 HOMO: -7.28993 LUMO: 0.11429 factor:1 | -1 (0.27467) | 1 | 1 |
| G: -5717.87902 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.82587 HOMO: -6.86271 LUMO: -1.03947 factor:1 | 1 (-0.58115) | -1 | -1 |
| G: -5717.87902 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.32110 HOMO: -6.55794 LUMO: -0.84900 factor:1 | 1 (-0.07638) | -1 | -1 |
| G: -5717.87902 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.89157 HOMO: -7.03686 LUMO: 0.11429 factor:1 | -1 (0.35315) | -1 | -1 |
| G: -5717.87902 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.78269 HOMO: -7.06952 LUMO: -0.96056 factor:1 | -1 (0.46202) | 1 | 1 |
| G: -5717.87902 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.78087 HOMO: -6.90897 LUMO: -0.99866 factor:1 | -1 (0.46385) | -1 | -1 |
| G: -5717.87902 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.82299 HOMO: -7.00693 LUMO: -0.83539 factor:1 | -1 (0.42172) | -1 | -1 |
| G: -5717.87902 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.69216 HOMO: -6.74298 LUMO: -0.85172 factor:1 | -1 (0.55255) | -1 | -1 |
| G: -5717.87902 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.46718 HOMO: -6.83822 LUMO: -1.07213 factor:1 | -1 (0.77754) | -1 | -1 |
| G: -5717.87902 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.89323 HOMO: -7.21918 LUMO: -1.55377 factor:1 | -1 (0.35149) | 1 | 1 |
| G: -5717.87902 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.52603 HOMO: -6.84094 LUMO: -1.09934 factor:1 | -1 (0.71868) | -1 | -1 |
| G: -5717.87902 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.36228 HOMO: -7.09129 LUMO: -0.85988 factor:1 | -1 (0.88244) | 1 | 1 |
| G: -5717.87902 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.58160 HOMO: -6.57971 LUMO: -2.27215 factor:1 | -1 (0.66311) | -1 | -1 |
| G: -5717.87902 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.59118 HOMO: -6.81373 LUMO: -1.86942 factor:1 | -1 (0.65354) | -1 | -1 |
| G: -5717.87902 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.79992 HOMO: -6.59060 LUMO: -2.30480 factor:1 | -1 (0.44480) | -1 | -1 |
| G: -5717.87902 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.87731 HOMO: -6.72938 LUMO: -1.23540 factor:1 | -1 (0.36741) | -1 | -1 |
| G: -5715.18379 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.16644 HOMO: -6.94707 LUMO: -2.62318 factor:1 | 1 (-1.61695) | -1 | -1 |
| G: -5715.18379 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.55948 HOMO: -7.28177 LUMO: -0.09796 factor:1 | 1 (-2.01000) | 1 | 1 |
| G: -5715.18379 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.40174 HOMO: -6.80013 LUMO: -0.79729 factor:1 | 1 (-0.85226) | -1 | -1 |
| G: -5715.18379 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.48163 HOMO: -7.26544 LUMO: 0.12789 factor:1 | 1 (-0.93215) | 1 | 1 |
| G: -5715.18379 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.37668 HOMO: -6.51713 LUMO: -0.49253 factor:1 | 1 (-0.82720) | -1 | -1 |
| G: -5715.18379 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.45962 HOMO: -6.68856 LUMO: -0.77280 factor:1 | 1 (-0.91014) | -1 | -1 |
| G: -5715.18379 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.50193 HOMO: -6.41100 LUMO: -0.70750 factor:1 | 1 (-0.95245) | -1 | -1 |
| G: -5715.18379 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.43216 HOMO: -7.56204 LUMO: 0.22041 factor:1 | 1 (-0.88268) | 1 | 1 |
| G: -5715.18379 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.47709 HOMO: -6.68312 LUMO: 1.30343 factor:1 | 1 (-0.92761) | -1 | -1 |
| G: -5715.18379 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.06097 HOMO: -7.24367 LUMO: 0.17415 factor:1 | 1 (-1.51148) | 1 | 1 |
| G: -5715.18379 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.17759 HOMO: -7.52395 LUMO: 1.16737 factor:1 | 1 (-1.62811) | 1 | 1 |
| G: -5715.18379 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.19719 HOMO: -6.89264 LUMO: 0.23130 factor:1 | 1 (-1.64770) | -1 | -1 |
| G: -5715.18379 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.54593 HOMO: -7.21102 LUMO: 0.19048 factor:1 | 1 (-1.99644) | 1 | 1 |
| G: -5715.18379 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.46677 HOMO: -7.08312 LUMO: 0.25034 factor:1 | 1 (-1.91729) | 1 | 1 |
| G: -5715.18379 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.26871 HOMO: -6.49536 LUMO: -0.65852 factor:1 | 1 (-0.71922) | -1 | -1 |
| G: -5715.18379 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.40876 HOMO: -6.85455 LUMO: 0.13606 factor:1 | 1 (-0.85928) | -1 | -1 |
| G: -5715.18379 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.11442 HOMO: -7.10217 LUMO: 0.35919 factor:1 | 1 (-0.56494) | 1 | 1 |
| G: -5715.18379 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.38253 HOMO: -7.77429 LUMO: 1.19186 factor:1 | 1 (-0.83305) | 1 | 1 |
| G: -5715.18379 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.39693 HOMO: -6.57427 LUMO: -0.50069 factor:1 | 1 (-0.84744) | -1 | -1 |
| G: -5715.18379 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.17667 HOMO: -7.36340 LUMO: 0.10068 factor:1 | 1 (-1.62719) | 1 | 1 |
| G: -5715.18379 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.87269 HOMO: -7.28177 LUMO: 0.15238 factor:1 | 1 (-1.32321) | 1 | 1 |
| G: -5715.18379 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.06785 HOMO: -6.86543 LUMO: -0.84355 factor:1 | 1 (-1.51837) | -1 | -1 |
| G: -5715.18379 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.19310 HOMO: -6.55794 LUMO: 1.39594 factor:1 | 1 (-1.64362) | -1 | -1 |
| G: -5715.18379 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.38095 HOMO: -6.26134 LUMO: 1.53744 factor:1 | 1 (-0.83147) | -1 | -1 |
| G: -5715.18379 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.44988 HOMO: -5.97562 LUMO: 1.42316 factor:1 | 1 (-0.90040) | -1 | -1 |
| G: -5715.18379 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.14434 HOMO: -6.65046 LUMO: 1.44492 factor:1 | 1 (-1.59486) | -1 | -1 |
| G: -5715.18379 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.06932 HOMO: -6.92258 LUMO: 0.17415 factor:1 | 1 (-1.51984) | -1 | -1 |
| G: -5715.18379 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.14551 HOMO: -7.40966 LUMO: 0.19592 factor:1 | 1 (-1.59603) | 1 | 1 |
| G: -5715.18379 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.44173 HOMO: -7.17564 LUMO: 0.16871 factor:1 | 1 (-1.89225) | 1 | 1 |
| G: -5715.18379 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.37505 HOMO: -7.46953 LUMO: 0.22313 factor:1 | 1 (-0.82557) | 1 | 1 |
| G: -5715.18379 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.12941 HOMO: -6.13345 LUMO: 1.85854 factor:1 | 1 (-0.57993) | -1 | -1 |
| G: -5715.18379 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.35845 HOMO: -6.99333 LUMO: -1.65717 factor:1 | 1 (-0.80897) | -1 | -1 |
| G: -5715.18379 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.33594 HOMO: -6.93074 LUMO: -1.79323 factor:1 | 1 (-0.78646) | -1 | -1 |
| G: -5715.18379 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.39290 HOMO: -6.87904 LUMO: -1.79323 factor:1 | 1 (-0.84342) | -1 | -1 |
| G: -5715.18379 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.45965 HOMO: -6.84094 LUMO: 0.66940 factor:1 | 1 (-0.91017) | -1 | -1 |
| G: -5715.18379 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.32109 HOMO: -7.13210 LUMO: -1.17553 factor:1 | 1 (-0.77161) | 1 | 1 |
| G: -5715.18379 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.38065 HOMO: -6.52801 LUMO: -2.23678 factor:1 | 1 (-0.83117) | -1 | -1 |
| G: -5715.18379 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.42474 HOMO: -6.81917 LUMO: -1.86398 factor:1 | 1 (-0.87525) | -1 | -1 |
| G: -5715.18379 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.07931 HOMO: -7.30626 LUMO: -1.66806 factor:1 | 1 (-1.52982) | 1 | 1 |
| G: -5715.18379 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.87049 HOMO: -6.98516 LUMO: -1.40683 factor:1 | 1 (-1.32100) | -1 | -1 |
| G: -5715.18379 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.18203 HOMO: -6.95523 LUMO: -0.97145 factor:1 | 1 (-1.63255) | -1 | -1 |
| G: -5715.18379 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.18187 HOMO: -6.83278 LUMO: -2.68848 factor:1 | 1 (-0.63239) | -1 | -1 |
| G: -5715.18379 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.32876 HOMO: -7.25456 LUMO: -2.97420 factor:1 | 1 (-0.77928) | -1 | -1 |
| G: -5715.18379 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.05128 HOMO: -6.80557 LUMO: -2.65039 factor:1 | 1 (-1.50180) | -1 | -1 |
| G: -5715.18379 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.06167 HOMO: -7.10489 LUMO: 0.77008 factor:1 | 1 (-1.51219) | 1 | -1 |
| G: -5715.18379 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.10853 HOMO: -7.28993 LUMO: -1.06124 factor:1 | 1 (-1.55905) | 1 | 1 |
| G: -5715.18379 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.10497 HOMO: -7.11578 LUMO: -1.10206 factor:1 | 1 (-1.55548) | 1 | 1 |
| G: -5715.18379 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.23483 HOMO: -6.91713 LUMO: -1.36329 factor:1 | 1 (-0.68535) | -1 | -1 |
| G: -5715.18379 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.06778 HOMO: -7.07224 LUMO: 0.51974 factor:1 | 1 (-0.51830) | 1 | 1 |
| G: -5715.18379 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.17567 HOMO: -7.22734 LUMO: -0.93335 factor:1 | 1 (-0.62619) | 1 | 1 |
| G: -5715.18379 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11979.99120 HOMO: -7.19469 LUMO: -0.96600 factor:1 | 1 (-0.44172) | 1 | 1 |
| G: -5715.18379 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.15401 HOMO: -6.93890 LUMO: -0.66940 factor:1 | 1 (-0.60453) | -1 | -1 |
| G: -5715.18379 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.12820 HOMO: -7.09673 LUMO: -1.05852 factor:1 | 1 (-1.57872) | 1 | 1 |
| G: -5715.18379 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.10271 HOMO: -7.19197 LUMO: -2.26943 factor:1 | 1 (-1.55323) | -1 | -1 |
| G: -5715.18379 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.34707 HOMO: -6.90081 LUMO: -2.64767 factor:1 | 1 (-0.79759) | -1 | -1 |
| G: -5715.18379 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.26558 HOMO: -6.93890 LUMO: -2.65039 factor:1 | 1 (-0.71609) | -1 | -1 |
| G: -5715.18379 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.40797 HOMO: -6.80013 LUMO: -2.54154 factor:1 | 1 (-0.85849) | -1 | -1 |
| G: -5715.18379 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.08408 HOMO: -6.68040 LUMO: -0.89798 factor:1 | 1 (-0.53459) | -1 | -1 |
| G: -5715.18379 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.12753 HOMO: -7.01782 LUMO: -1.09662 factor:1 | 1 (-0.57805) | -1 | -1 |
| G: -5715.18379 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.07131 HOMO: -6.58516 LUMO: -0.83539 factor:1 | 1 (-0.52183) | -1 | -1 |
| G: -5715.18379 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.21692 HOMO: -7.46953 LUMO: 0.06259 factor:1 | 1 (-0.66744) | 1 | 1 |
| G: -5715.18379 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.15626 HOMO: -6.96884 LUMO: -0.99866 factor:1 | 1 (-1.60678) | -1 | -1 |
| G: -5715.18379 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.27581 HOMO: -7.29809 LUMO: -0.19320 factor:1 | 1 (-0.72633) | 1 | 1 |
| G: -5715.18379 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.23864 HOMO: -6.86271 LUMO: 0.04082 factor:1 | 1 (-0.68916) | -1 | -1 |
| G: -5715.18379 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.03199 HOMO: -6.36746 LUMO: -1.02587 factor:1 | 1 (-0.48251) | -1 | -1 |
| G: -5715.18379 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.34248 HOMO: -7.15659 LUMO: -1.25989 factor:1 | 1 (-0.79299) | 1 | 1 |
| G: -5715.18379 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.34841 HOMO: -6.69128 LUMO: -0.59865 factor:1 | 1 (-0.79893) | -1 | -1 |
| G: -5715.18379 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.97770 HOMO: -7.09129 LUMO: -1.08573 factor:1 | 1 (-1.42822) | 1 | 1 |
| G: -5715.18379 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.16557 HOMO: -6.64502 LUMO: -0.66396 factor:1 | 1 (-1.61608) | -1 | -1 |
| G: -5715.18379 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.92314 HOMO: -6.93346 LUMO: -0.87349 factor:1 | 1 (-1.37366) | -1 | -1 |
| G: -5715.18379 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.81595 HOMO: -6.77019 LUMO: -0.87349 factor:1 | 1 (-1.26647) | -1 | -1 |
| G: -5715.18379 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.97645 HOMO: -6.59060 LUMO: -0.82995 factor:1 | 1 (-1.42697) | -1 | -1 |
| G: -5715.18379 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.09714 HOMO: -7.17564 LUMO: -1.08846 factor:1 | 1 (-0.54766) | 1 | 1 |
| G: -5715.18379 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.03711 HOMO: -7.27088 LUMO: -1.18642 factor:1 | 1 (-0.48763) | 1 | 1 |
| G: -5715.18379 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.18274 HOMO: -7.06680 LUMO: -1.13199 factor:1 | 1 (-0.63326) | 1 | 1 |
| G: -5715.18379 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11979.94688 HOMO: -7.21918 LUMO: -1.03947 factor:1 | 1 (-0.39740) | 1 | 1 |
| G: -5715.18379 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.16873 HOMO: -7.26000 LUMO: -0.11973 factor:1 | 1 (-0.61925) | 1 | 1 |
| G: -5715.18379 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.29230 HOMO: -6.77564 LUMO: 0.23402 factor:1 | 1 (-0.74282) | -1 | -1 |
| G: -5715.18379 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.06818 HOMO: -7.07224 LUMO: -0.75648 factor:1 | 1 (-0.51870) | 1 | 1 |
| G: -5715.18379 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.32381 HOMO: -7.45048 LUMO: 0.18232 factor:1 | 1 (-0.77433) | 1 | 1 |
| G: -5715.18379 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.32392 HOMO: -7.48313 LUMO: 0.15238 factor:1 | 1 (-0.77444) | 1 | 1 |
| G: -5715.18379 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.33246 HOMO: -6.60692 LUMO: -0.50885 factor:1 | 1 (-0.78298) | -1 | -1 |
| G: -5715.18379 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11979.99673 HOMO: -6.62869 LUMO: -0.60954 factor:1 | 1 (-0.44725) | -1 | -1 |
| G: -5715.18379 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.83220 HOMO: -7.40422 LUMO: -1.28982 factor:1 | 1 (-1.28272) | 1 | 1 |
| G: -5715.18379 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.93138 HOMO: -6.75114 LUMO: -1.23268 factor:1 | 1 (-1.38190) | -1 | -1 |
| G: -5715.18379 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.96311 HOMO: -6.84638 LUMO: -0.73199 factor:1 | 1 (-1.41363) | -1 | -1 |
| G: -5715.18379 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.21961 HOMO: -6.79196 LUMO: -1.43676 factor:1 | 1 (-1.67013) | -1 | -1 |
| G: -5715.18379 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.61309 HOMO: -7.00965 LUMO: -1.37690 factor:1 | 1 (-1.06361) | -1 | -1 |
| G: -5715.18379 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.72425 HOMO: -6.97972 LUMO: -1.58098 factor:1 | 1 (-1.17477) | -1 | -1 |
| G: -5715.18379 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.05046 HOMO: -6.91169 LUMO: -1.48574 factor:1 | 1 (-1.50098) | -1 | -1 |
| G: -5715.18379 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.10687 HOMO: -6.90081 LUMO: -1.30343 factor:1 | 1 (-1.55739) | -1 | -1 |
| G: -5715.18379 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.94725 HOMO: -6.78652 LUMO: -1.51840 factor:1 | 1 (-1.39777) | -1 | -1 |
| G: -5715.18379 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.06056 HOMO: -6.84638 LUMO: -1.15104 factor:1 | 1 (-1.51108) | -1 | -1 |
| G: -5715.18379 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.94787 HOMO: -6.61237 LUMO: -0.89798 factor:1 | 1 (-1.39839) | -1 | -1 |
| G: -5715.18379 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.12141 HOMO: -7.16204 LUMO: -1.30070 factor:1 | 1 (-0.57193) | 1 | 1 |
| G: -5715.18379 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.12152 HOMO: -7.32803 LUMO: 0.14694 factor:1 | 1 (-0.57204) | 1 | 1 |
| G: -5715.18379 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11979.94160 HOMO: -6.99877 LUMO: -0.87621 factor:1 | 1 (-0.39212) | -1 | -1 |
| G: -5715.18379 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.17771 HOMO: -6.99877 LUMO: -0.97145 factor:1 | 1 (-0.62823) | -1 | -1 |
| G: -5715.18379 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.16944 HOMO: -7.08040 LUMO: -1.09662 factor:1 | 1 (-0.61996) | 1 | 1 |
| G: -5715.18379 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.01482 HOMO: -6.90897 LUMO: -1.14016 factor:1 | 1 (-0.46534) | -1 | -1 |
| G: -5715.18379 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.11053 HOMO: -6.68312 LUMO: -0.74831 factor:1 | 1 (-0.56104) | -1 | -1 |
| G: -5715.18379 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.15406 HOMO: -6.99061 LUMO: -0.86804 factor:1 | 1 (-0.60458) | -1 | -1 |
| G: -5715.18379 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.37303 HOMO: -7.10761 LUMO: -1.18642 factor:1 | 1 (-0.82355) | 1 | 1 |
| G: -5715.18379 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.44563 HOMO: -6.79196 LUMO: -0.71294 factor:1 | 1 (-0.89615) | -1 | -1 |
| G: -5715.18379 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.22470 HOMO: -6.86271 LUMO: -0.81362 factor:1 | 1 (-0.67522) | -1 | -1 |
| G: -5715.18379 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.27466 HOMO: -7.01510 LUMO: -0.99322 factor:1 | 1 (-0.72518) | -1 | -1 |
| G: -5715.18379 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.06252 HOMO: -6.88720 LUMO: -0.87893 factor:1 | 1 (-0.51304) | -1 | -1 |
| G: -5715.18379 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.06952 HOMO: -6.88448 LUMO: 0.22041 factor:1 | 1 (-0.52004) | -1 | -1 |
| G: -5715.18379 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.27730 HOMO: -7.55932 LUMO: 1.12111 factor:1 | 1 (-0.72782) | 1 | 1 |
| G: -5715.18379 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.12530 HOMO: -6.46815 LUMO: -0.86260 factor:1 | 1 (-0.57582) | -1 | -1 |
| G: -5715.18379 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.28242 HOMO: -7.13755 LUMO: 0.23130 factor:1 | 1 (-0.73294) | 1 | 1 |
| G: -5715.18379 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11979.95452 HOMO: -6.78924 LUMO: 1.51023 factor:1 | 1 (-0.40504) | -1 | -1 |
| G: -5715.18379 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.92567 HOMO: -6.48992 LUMO: 1.74969 factor:1 | 1 (-1.37619) | -1 | -1 |
| G: -5715.18379 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.84559 HOMO: -6.78380 LUMO: 1.81500 factor:1 | 1 (-1.29611) | -1 | -1 |
| G: -5715.18379 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.37127 HOMO: -6.49536 LUMO: 1.70615 factor:1 | 1 (-0.82178) | -1 | -1 |
| G: -5715.18379 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.80148 HOMO: -6.38651 LUMO: 1.44492 factor:1 | 1 (-1.25200) | -1 | -1 |
| G: -5715.18379 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.93666 HOMO: -6.83822 LUMO: 1.38234 factor:1 | 1 (-1.38718) | -1 | -1 |
| G: -5715.18379 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.74569 HOMO: -6.01644 LUMO: 1.20274 factor:1 | 1 (-1.19621) | -1 | -1 |
| G: -5715.18379 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.10067 HOMO: -6.18243 LUMO: 1.77962 factor:1 | 1 (-1.55119) | -1 | -1 |
| G: -5715.18379 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.09189 HOMO: -6.81917 LUMO: -1.01771 factor:1 | 1 (-0.54240) | -1 | -1 |
| G: -5715.18379 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11979.83479 HOMO: -6.61237 LUMO: -0.91702 factor:1 | 1 (-0.28531) | -1 | -1 |
| G: -5715.18379 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.07235 HOMO: -6.84094 LUMO: -0.84900 factor:1 | 1 (-0.52287) | -1 | -1 |
| G: -5715.18379 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.26324 HOMO: -6.81917 LUMO: -1.01771 factor:1 | 1 (-0.71375) | -1 | -1 |
| G: -5715.18379 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.29662 HOMO: -7.86953 LUMO: 1.16737 factor:1 | 1 (-0.74714) | 1 | 1 |
| G: -5715.18379 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.02228 HOMO: -7.40694 LUMO: 0.11429 factor:1 | 1 (-0.47280) | 1 | 1 |
| G: -5715.18379 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.07678 HOMO: -6.70489 LUMO: -0.65035 factor:1 | 1 (-0.52730) | -1 | -1 |
| G: -5715.18379 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.21232 HOMO: -7.23279 LUMO: 0.33470 factor:1 | 1 (-0.66284) | 1 | 1 |
| G: -5715.18379 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.24008 HOMO: -7.17020 LUMO: 0.41361 factor:1 | 1 (-0.69060) | 1 | 1 |
| G: -5715.18379 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.15779 HOMO: -6.90353 LUMO: -0.90070 factor:1 | 1 (-0.60831) | -1 | -1 |
| G: -5715.18379 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.59576 HOMO: -7.39061 LUMO: 0.17687 factor:1 | 1 (-1.04628) | 1 | 1 |
| G: -5715.18379 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.63203 HOMO: -7.16748 LUMO: 0.42178 factor:1 | 1 (-1.08255) | 1 | 1 |
| G: -5715.18379 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11979.87771 HOMO: -7.36884 LUMO: -1.11295 factor:1 | 1 (-0.32822) | 1 | 1 |
| G: -5715.18379 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11979.76698 HOMO: -7.33347 LUMO: 0.33198 factor:1 | 1 (-0.21750) | 1 | 1 |
| G: -5715.18379 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11979.79308 HOMO: -7.31986 LUMO: -0.83539 factor:1 | 1 (-0.24360) | 1 | 1 |
| G: -5715.18379 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.32316 HOMO: -7.31170 LUMO: 0.08708 factor:1 | 1 (-0.77367) | 1 | 1 |
| G: -5715.18379 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.13616 HOMO: -7.36884 LUMO: 0.38096 factor:1 | 1 (-0.58668) | 1 | 1 |
| G: -5715.18379 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.56362 HOMO: -6.99333 LUMO: 1.74153 factor:1 | 1 (-1.01414) | -1 | -1 |
| G: -5715.18379 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.35080 HOMO: -6.94435 LUMO: 1.74969 factor:1 | 1 (-0.80132) | -1 | -1 |
| G: -5715.18379 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.71799 HOMO: -7.02598 LUMO: 1.43404 factor:1 | 1 (-1.16851) | -1 | -1 |
| G: -5715.18379 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.56926 HOMO: -6.41100 LUMO: 1.62996 factor:1 | 1 (-1.01977) | -1 | -1 |
| G: -5715.18379 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.62542 HOMO: -6.57699 LUMO: 1.81228 factor:1 | 1 (-1.07594) | -1 | -1 |
| G: -5715.18379 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.87593 HOMO: -6.86543 LUMO: 1.49935 factor:1 | 1 (-1.32645) | -1 | -1 |
| G: -5715.18379 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.60283 HOMO: -6.91169 LUMO: -1.22451 factor:1 | 1 (-1.05335) | -1 | -1 |
| G: -5715.18379 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.92858 HOMO: -7.09945 LUMO: -1.23812 factor:1 | 1 (-1.37910) | 1 | 1 |
| G: -5715.18379 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.69971 HOMO: -7.48857 LUMO: 0.10340 factor:1 | 1 (-1.15023) | 1 | 1 |
| G: -5715.18379 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.28453 HOMO: -7.21918 LUMO: -0.06803 factor:1 | 1 (-1.73505) | 1 | 1 |
| G: -5715.18379 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.35683 HOMO: -6.34025 LUMO: -0.68845 factor:1 | 1 (-1.80735) | -1 | -1 |
| G: -5715.18379 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.48791 HOMO: -6.82734 LUMO: -0.77825 factor:1 | 1 (-1.93843) | -1 | -1 |
| G: -5715.18379 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.26780 HOMO: -6.92258 LUMO: -1.03675 factor:1 | 1 (-1.71832) | -1 | -1 |
| G: -5715.18379 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.08396 HOMO: -6.42461 LUMO: -0.95240 factor:1 | 1 (-1.53448) | -1 | -1 |
| G: -5715.18379 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.86955 HOMO: -6.96067 LUMO: -1.05036 factor:1 | 1 (-2.32007) | -1 | -1 |
| G: -5715.18379 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.76193 HOMO: -7.23551 LUMO: 0.12245 factor:1 | 1 (-2.21245) | 1 | 1 |
| G: -5715.18379 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.80563 HOMO: -6.85183 LUMO: 0.16055 factor:1 | 1 (-2.25615) | -1 | -1 |
| G: -5715.18379 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.57523 HOMO: -6.46815 LUMO: -0.89253 factor:1 | 1 (-2.02575) | -1 | -1 |
| G: -5715.18379 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.08512 HOMO: -7.23823 LUMO: -0.06259 factor:1 | 1 (-2.53564) | 1 | 1 |
| G: -5715.18379 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.57212 HOMO: -6.76475 LUMO: -0.99049 factor:1 | 1 (-3.02264) | -1 | -1 |
| G: -5715.18379 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.59425 HOMO: -7.14843 LUMO: -0.88165 factor:1 | 1 (-3.04476) | 1 | 1 |
| G: -5715.18379 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.52029 HOMO: -7.15659 LUMO: 0.20681 factor:1 | 1 (-1.97081) | 1 | 1 |
| G: -5715.18379 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.24735 HOMO: -7.11306 LUMO: 0.14150 factor:1 | 1 (-2.69787) | 1 | 1 |
| G: -5715.18379 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.54334 HOMO: -6.67223 LUMO: -0.86260 factor:1 | 1 (-1.99386) | -1 | -1 |
| G: -5715.18379 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.34265 HOMO: -6.92530 LUMO: 0.30749 factor:1 | 1 (-2.79317) | -1 | -1 |
| G: -5715.18379 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11983.03869 HOMO: -6.50624 LUMO: -0.70477 factor:1 | 1 (-3.48921) | -1 | -1 |
| G: -5715.18379 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.38360 HOMO: -7.35524 LUMO: 0.75103 factor:1 | 1 (-2.83412) | 1 | 1 |
| G: -5715.18379 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.09260 HOMO: -7.07768 LUMO: -0.26939 factor:1 | 1 (-2.54312) | 1 | 1 |
| G: -5715.18379 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.85608 HOMO: -7.15932 LUMO: 0.42450 factor:1 | 1 (-2.30660) | 1 | 1 |
| G: -5715.18379 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.88082 HOMO: -7.46136 LUMO: 0.04626 factor:1 | 1 (-2.33134) | 1 | 1 |
| G: -5715.18379 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.56136 HOMO: -7.05047 LUMO: -1.06669 factor:1 | 1 (-2.01187) | -1 | -1 |
| G: -5715.18379 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.69792 HOMO: -6.66951 LUMO: -0.99322 factor:1 | 1 (-3.14844) | -1 | -1 |
| G: -5715.18379 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.72524 HOMO: -7.01782 LUMO: -1.08846 factor:1 | 1 (-3.17576) | -1 | -1 |
| G: -5715.18379 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.79396 HOMO: -7.03959 LUMO: -1.15376 factor:1 | 1 (-2.24448) | -1 | -1 |
| G: -5715.18379 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.70152 HOMO: -6.68856 LUMO: 1.61364 factor:1 | 1 (-2.15204) | -1 | -1 |
| G: -5715.18379 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.75580 HOMO: -6.53345 LUMO: 1.60275 factor:1 | 1 (-3.20632) | -1 | -1 |
| G: -5715.18379 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.53906 HOMO: -6.73482 LUMO: 1.86398 factor:1 | 1 (-2.98958) | -1 | -1 |
| G: -5715.18379 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.10088 HOMO: -6.87632 LUMO: 1.59731 factor:1 | 1 (-1.55140) | -1 | -1 |
| G: -5715.18379 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.92581 HOMO: -6.31848 LUMO: 2.12521 factor:1 | 1 (-1.37632) | -1 | -1 |
| G: -5715.18379 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.96781 HOMO: -6.35114 LUMO: 1.71432 factor:1 | 1 (-2.41833) | -1 | -1 |
| G: -5715.18379 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.80639 HOMO: -6.34842 LUMO: 1.92929 factor:1 | 1 (-2.25691) | -1 | -1 |
| G: -5715.18379 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.00760 HOMO: -6.14977 LUMO: 1.78235 factor:1 | 1 (-1.45812) | -1 | -1 |
| G: -5715.18379 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.85057 HOMO: -6.31032 LUMO: 1.51567 factor:1 | 1 (-1.30109) | -1 | -1 |
| G: -5715.18379 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.80172 HOMO: -6.25862 LUMO: 1.75241 factor:1 | 1 (-1.25224) | -1 | -1 |
| G: -5715.18379 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.54389 HOMO: -6.49264 LUMO: 1.66806 factor:1 | 1 (-0.99441) | -1 | -1 |
| G: -5715.18379 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.88797 HOMO: -6.28311 LUMO: 1.60003 factor:1 | 1 (-2.33849) | -1 | -1 |
| G: -5715.18379 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.77407 HOMO: -7.13210 LUMO: -0.04354 factor:1 | 1 (-2.22459) | 1 | 1 |
| G: -5715.18379 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.38418 HOMO: -7.35252 LUMO: 0.03537 factor:1 | 1 (-1.83470) | 1 | 1 |
| G: -5715.18379 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.99304 HOMO: -6.58243 LUMO: -0.48980 factor:1 | 1 (-2.44356) | -1 | -1 |
| G: -5715.18379 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.87694 HOMO: -6.90081 LUMO: -0.05442 factor:1 | 1 (-3.32746) | -1 | -1 |
| G: -5715.18379 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11983.42923 HOMO: -7.22734 LUMO: 0.17143 factor:1 | 1 (-3.87974) | 1 | 1 |
| G: -5715.18379 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11983.50983 HOMO: -7.13210 LUMO: -0.99866 factor:1 | 1 (-3.96035) | 1 | 1 |
| G: -5715.18379 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.39972 HOMO: -7.39878 LUMO: 0.13334 factor:1 | 1 (-1.85024) | 1 | 1 |
| G: -5715.18379 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11983.51698 HOMO: -7.04503 LUMO: -0.89798 factor:1 | 1 (-3.96750) | -1 | -1 |
| G: -5715.18379 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.12507 HOMO: -6.95523 LUMO: -1.07213 factor:1 | 1 (-2.57558) | -1 | -1 |
| G: -5715.18379 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.33674 HOMO: -6.75114 LUMO: -1.28438 factor:1 | 1 (-2.78726) | -1 | -1 |
| G: -5715.18379 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.38238 HOMO: -6.75114 LUMO: -0.11701 factor:1 | 1 (-2.83290) | -1 | -1 |
| G: -5715.18379 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11983.07374 HOMO: -6.83278 LUMO: -0.01633 factor:1 | 1 (-3.52426) | -1 | -1 |
| G: -5715.18379 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.40532 HOMO: -6.93890 LUMO: -0.88981 factor:1 | 1 (-2.85583) | -1 | -1 |
| G: -5715.18379 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11983.09581 HOMO: -7.07224 LUMO: -1.08573 factor:1 | 1 (-3.54632) | 1 | 1 |
| G: -5715.18379 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.56956 HOMO: -6.99877 LUMO: -0.95240 factor:1 | 1 (-3.02008) | -1 | -1 |
| G: -5715.18379 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.56886 HOMO: -7.09129 LUMO: 0.35375 factor:1 | 1 (-3.01938) | 1 | 1 |
| G: -5715.18379 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.71169 HOMO: -7.09401 LUMO: 0.04354 factor:1 | 1 (-3.16221) | 1 | 1 |
| G: -5715.18379 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.61152 HOMO: -6.85183 LUMO: -0.68573 factor:1 | 1 (-3.06204) | -1 | -1 |
| G: -5715.18379 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.47626 HOMO: -6.83006 LUMO: -0.58777 factor:1 | 1 (-2.92678) | -1 | -1 |
| G: -5715.18379 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11983.11948 HOMO: -7.40422 LUMO: 0.17687 factor:1 | 1 (-3.57000) | 1 | 1 |
| G: -5715.18379 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11983.18215 HOMO: -7.15932 LUMO: 0.10340 factor:1 | 1 (-3.63267) | 1 | 1 |
| G: -5715.18379 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.99833 HOMO: -7.03414 LUMO: -0.19592 factor:1 | 1 (-3.44885) | -1 | -1 |
| G: -5715.18379 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.85074 HOMO: -6.48447 LUMO: -0.36191 factor:1 | 1 (-3.30126) | -1 | -1 |
| G: -5715.18379 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11983.23603 HOMO: -7.49402 LUMO: 0.11429 factor:1 | 1 (-3.68654) | 1 | 1 |
| G: -5715.18379 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11983.20392 HOMO: -7.01237 LUMO: -1.06397 factor:1 | 1 (-3.65443) | -1 | -1 |
| G: -5715.18379 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.36703 HOMO: -6.67223 LUMO: -1.07213 factor:1 | 1 (-2.81755) | -1 | -1 |
| G: -5715.18379 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.55713 HOMO: -7.38789 LUMO: -1.15376 factor:1 | 1 (-3.00765) | 1 | 1 |
| G: -5715.18379 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.68538 HOMO: -6.42461 LUMO: -1.23812 factor:1 | 1 (-3.13589) | -1 | -1 |
| G: -5715.18379 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.60954 HOMO: -7.36884 LUMO: -1.19186 factor:1 | 1 (-3.06006) | 1 | 1 |
| G: -5715.18379 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.59367 HOMO: -6.65591 LUMO: 0.07075 factor:1 | 1 (-3.04419) | -1 | -1 |
| G: -5715.18379 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.68843 HOMO: -7.39061 LUMO: -0.16871 factor:1 | 1 (-2.13895) | 1 | 1 |
| G: -5715.18379 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.42877 HOMO: -6.90353 LUMO: -0.96056 factor:1 | 1 (-2.87929) | -1 | -1 |
| G: -5715.18379 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.44739 HOMO: -7.42054 LUMO: 0.19048 factor:1 | 1 (-2.89790) | 1 | 1 |
| G: -5715.18379 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.30050 HOMO: -7.40150 LUMO: 0.35647 factor:1 | 1 (-2.75102) | 1 | 1 |
| G: -5715.18379 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.48333 HOMO: -6.56067 LUMO: -0.96056 factor:1 | 1 (-2.93385) | -1 | -1 |
| G: -5715.18379 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.48080 HOMO: -6.89809 LUMO: -0.81090 factor:1 | 1 (-2.93132) | -1 | -1 |
| G: -5715.18379 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.58875 HOMO: -6.91986 LUMO: -0.84900 factor:1 | 1 (-3.03927) | -1 | -1 |
| G: -5715.18379 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.02896 HOMO: -6.61509 LUMO: -0.62042 factor:1 | 1 (-2.47947) | -1 | -1 |
| G: -5715.18379 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.67732 HOMO: -6.58243 LUMO: -0.65579 factor:1 | 1 (-3.12784) | -1 | -1 |
| G: -5715.18379 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11983.13322 HOMO: -6.52257 LUMO: -0.92519 factor:1 | 1 (-3.58374) | -1 | -1 |
| G: -5715.18379 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.99284 HOMO: -6.69128 LUMO: 1.49118 factor:1 | 1 (-3.44336) | -1 | -1 |
| G: -5715.18379 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.98938 HOMO: -7.02870 LUMO: 1.67894 factor:1 | 1 (-3.43990) | -1 | -1 |
| G: -5715.18379 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11983.06887 HOMO: -6.88720 LUMO: 1.68711 factor:1 | 1 (-3.51938) | -1 | -1 |
| G: -5715.18379 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.26116 HOMO: -5.89943 LUMO: 1.03675 factor:1 | 1 (-1.71168) | -1 | -1 |
| G: -5715.18379 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.00480 HOMO: -6.40556 LUMO: 1.14560 factor:1 | 1 (-1.45532) | -1 | -1 |
| G: -5715.18379 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.49729 HOMO: -6.51168 LUMO: 1.48030 factor:1 | 1 (-2.94781) | -1 | -1 |
| G: -5715.18379 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11983.13151 HOMO: -6.64502 LUMO: 1.91568 factor:1 | 1 (-3.58203) | -1 | -1 |
| G: -5715.18379 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11983.29099 HOMO: -6.47903 LUMO: 1.91296 factor:1 | 1 (-3.74151) | -1 | -1 |
| G: -5715.18379 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.52595 HOMO: -6.34297 LUMO: 1.91840 factor:1 | 1 (-1.97647) | -1 | -1 |
| G: -5715.18379 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.18629 HOMO: -6.89809 LUMO: 1.82861 factor:1 | 1 (-2.63681) | -1 | -1 |
| G: -5715.18379 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.49901 HOMO: -6.10079 LUMO: 1.62996 factor:1 | 1 (-2.94952) | -1 | -1 |
| G: -5715.18379 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.22061 HOMO: -7.16476 LUMO: -0.92247 factor:1 | 1 (-2.67112) | 1 | 1 |
| G: -5715.18379 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.42254 HOMO: -7.10489 LUMO: -0.95784 factor:1 | 1 (-2.87306) | 1 | 1 |
| G: -5715.18379 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.89131 HOMO: -6.76475 LUMO: -0.99866 factor:1 | 1 (-3.34183) | -1 | -1 |
| G: -5715.18379 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.93877 HOMO: -6.81373 LUMO: -1.05036 factor:1 | 1 (-3.38929) | -1 | -1 |
| G: -5715.18379 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.52586 HOMO: -6.90081 LUMO: -1.03947 factor:1 | 1 (-2.97638) | -1 | -1 |
| G: -5715.18379 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.52369 HOMO: -7.06952 LUMO: -0.91702 factor:1 | 1 (-2.97420) | 1 | 1 |
| G: -5715.18379 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.57232 HOMO: -6.73482 LUMO: -0.94151 factor:1 | 1 (-2.02284) | -1 | -1 |
| G: -5715.18379 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.28806 HOMO: -6.99605 LUMO: -1.04764 factor:1 | 1 (-2.73858) | -1 | -1 |
| G: -5715.18379 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.82794 HOMO: -7.03686 LUMO: -0.93335 factor:1 | 1 (-3.27845) | -1 | -1 |
| G: -5715.18379 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.47803 HOMO: -6.81101 LUMO: -0.95240 factor:1 | 1 (-2.92854) | -1 | -1 |
| G: -5715.18379 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.59743 HOMO: -6.83822 LUMO: -0.65307 factor:1 | 1 (-3.04795) | -1 | -1 |
| G: -5715.18379 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.22959 HOMO: -7.05319 LUMO: -0.81634 factor:1 | 1 (-2.68010) | -1 | -1 |
| G: -5715.18379 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.36621 HOMO: -7.57565 LUMO: 0.19048 factor:1 | 1 (-2.81673) | 1 | 1 |
| G: -5715.18379 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.44510 HOMO: -6.56067 LUMO: -0.50613 factor:1 | 1 (-2.89562) | -1 | -1 |
| G: -5715.18379 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.19693 HOMO: -6.74298 LUMO: -0.70477 factor:1 | 1 (-2.64745) | -1 | -1 |
| G: -5715.18379 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.88995 HOMO: -7.02054 LUMO: 0.03537 factor:1 | 1 (-3.34047) | -1 | -1 |
| G: -5715.18379 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11983.05395 HOMO: -7.33347 LUMO: -0.17960 factor:1 | 1 (-3.50447) | 1 | 1 |
| G: -5715.18379 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.90628 HOMO: -6.98244 LUMO: -0.88165 factor:1 | 1 (-3.35680) | -1 | -1 |
| G: -5715.18379 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11983.60458 HOMO: -7.14843 LUMO: -1.19730 factor:1 | 1 (-4.05510) | 1 | 1 |
| G: -5715.18379 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11983.01806 HOMO: -7.17564 LUMO: -1.21907 factor:1 | 1 (-3.46858) | 1 | 1 |
| G: -5715.18379 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.91637 HOMO: -6.74026 LUMO: -0.86532 factor:1 | 1 (-3.36689) | -1 | -1 |
| G: -5715.18379 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.73536 HOMO: -6.82462 LUMO: -1.24084 factor:1 | 1 (-3.18588) | -1 | -1 |
| G: -5715.18379 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.60049 HOMO: -6.78924 LUMO: -0.70477 factor:1 | 1 (-2.05100) | -1 | -1 |
| G: -5715.18379 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.61357 HOMO: -7.41238 LUMO: 0.05987 factor:1 | 1 (-2.06409) | 1 | 1 |
| G: -5715.18379 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.39212 HOMO: -6.75931 LUMO: 0.02721 factor:1 | 1 (-2.84264) | -1 | -1 |
| G: -5715.18379 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.32102 HOMO: -6.28583 LUMO: -0.93063 factor:1 | 1 (-2.77153) | -1 | -1 |
| G: -5715.18379 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.22526 HOMO: -6.69128 LUMO: -0.83539 factor:1 | 1 (-2.67578) | -1 | -1 |
| G: -5715.18379 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.21369 HOMO: -7.22190 LUMO: 0.01361 factor:1 | 1 (-2.66421) | 1 | 1 |
| G: -5715.18379 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.19810 HOMO: -6.95251 LUMO: -1.09934 factor:1 | 1 (-2.64862) | -1 | -1 |
| G: -5715.18379 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.41049 HOMO: -6.75387 LUMO: -0.90614 factor:1 | 1 (-2.86101) | -1 | -1 |
| G: -5715.18379 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.35990 HOMO: -7.48585 LUMO: 0.05987 factor:1 | 1 (-2.81042) | 1 | 1 |
| G: -5715.18379 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.81243 HOMO: -6.92802 LUMO: -0.66940 factor:1 | 1 (-3.26294) | -1 | -1 |
| G: -5715.18379 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.32134 HOMO: -7.29537 LUMO: -0.14150 factor:1 | 1 (-2.77186) | 1 | 1 |
| G: -5715.18379 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.31710 HOMO: -6.57155 LUMO: -0.86804 factor:1 | 1 (-2.76762) | -1 | -1 |
| G: -5715.18379 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.40250 HOMO: -6.87632 LUMO: -0.77825 factor:1 | 1 (-1.85301) | -1 | -1 |
| G: -5715.18379 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.39229 HOMO: -6.45998 LUMO: -0.31565 factor:1 | 1 (-1.84281) | -1 | -1 |
| G: -5715.18379 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.27441 HOMO: -7.51306 LUMO: 0.05714 factor:1 | 1 (-1.72493) | 1 | 1 |
| G: -5715.18379 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.30306 HOMO: -6.86271 LUMO: -0.00816 factor:1 | 1 (-2.75357) | -1 | -1 |
| G: -5715.18379 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.10626 HOMO: -6.43277 LUMO: -1.07485 factor:1 | 1 (-2.55678) | -1 | -1 |
| G: -5715.18379 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.34300 HOMO: -6.78108 LUMO: -0.81362 factor:1 | 1 (-2.79352) | -1 | -1 |
| G: -5715.18379 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.16463 HOMO: -6.88448 LUMO: 1.21907 factor:1 | 1 (-2.61515) | -1 | -1 |
| G: -5715.18379 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.17075 HOMO: -6.97700 LUMO: 1.44765 factor:1 | 1 (-2.62127) | -1 | -1 |
| G: -5715.18379 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.77017 HOMO: -6.89537 LUMO: 2.12249 factor:1 | 1 (-3.22069) | -1 | -1 |
| G: -5715.18379 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.31225 HOMO: -6.28311 LUMO: 1.45037 factor:1 | 1 (-2.76277) | -1 | -1 |
| G: -5715.18379 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.08463 HOMO: -6.55522 LUMO: 1.39867 factor:1 | 1 (-2.53515) | -1 | -1 |
| G: -5715.18379 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.20730 HOMO: -6.46815 LUMO: 1.50207 factor:1 | 1 (-2.65782) | -1 | -1 |
| G: -5715.18379 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.19767 HOMO: -6.43549 LUMO: 2.17419 factor:1 | 1 (-2.64818) | -1 | -1 |
| G: -5715.18379 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.74753 HOMO: -6.99333 LUMO: 1.87214 factor:1 | 1 (-3.19805) | -1 | -1 |
| G: -5715.18379 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11983.54349 HOMO: -6.65591 LUMO: 1.37962 factor:1 | 1 (-3.99401) | -1 | -1 |
| G: -5715.18379 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11983.55219 HOMO: -6.82734 LUMO: 1.55649 factor:1 | 1 (-4.00271) | -1 | -1 |
| G: -5715.18379 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.56058 HOMO: -6.71849 LUMO: 1.36057 factor:1 | 1 (-3.01110) | -1 | -1 |
| G: -5715.18379 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.36391 HOMO: -6.79468 LUMO: 1.82044 factor:1 | 1 (-1.81443) | -1 | -1 |
| G: -5715.18379 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.08665 HOMO: -6.61237 LUMO: 1.15104 factor:1 | 1 (-1.53717) | -1 | -1 |
| G: -5715.18379 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.18452 HOMO: -6.62053 LUMO: 2.33474 factor:1 | 1 (-2.63504) | -1 | -1 |
| G: -5715.18379 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.87728 HOMO: -6.55794 LUMO: 1.65717 factor:1 | 1 (-2.32780) | -1 | -1 |
| G: -5715.18379 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.22186 HOMO: -6.85999 LUMO: 2.03813 factor:1 | 1 (-2.67238) | -1 | -1 |
| G: -5715.18379 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.06874 HOMO: -6.45726 LUMO: 1.28438 factor:1 | 1 (-2.51926) | -1 | -1 |
| G: -5715.18379 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.99755 HOMO: -6.23685 LUMO: 1.93201 factor:1 | 1 (-2.44807) | -1 | -1 |
| G: -5715.18379 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.71142 HOMO: -7.06680 LUMO: 1.86942 factor:1 | 1 (-3.16194) | 1 | 1 |
| G: -5715.18379 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.06708 HOMO: -6.89537 LUMO: 2.17147 factor:1 | 1 (-2.51760) | -1 | -1 |
| G: -5715.18379 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.15130 HOMO: -6.80013 LUMO: 1.78779 factor:1 | 1 (-2.60182) | -1 | -1 |
| G: -5715.18379 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.12278 HOMO: -6.45726 LUMO: 1.58370 factor:1 | 1 (-2.57330) | -1 | -1 |
| G: -5715.18379 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.44831 HOMO: -6.52529 LUMO: 1.71976 factor:1 | 1 (-2.89883) | -1 | -1 |
| G: -5715.18379 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11983.26084 HOMO: -7.22462 LUMO: -1.18642 factor:1 | 1 (-3.71136) | 1 | 1 |
| G: -5715.18379 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.40031 HOMO: -7.18381 LUMO: -0.78641 factor:1 | 1 (-2.85083) | 1 | 1 |
| G: -5715.18379 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11983.16827 HOMO: -6.93346 LUMO: 1.65717 factor:1 | 1 (-3.61879) | -1 | -1 |
| G: -5715.18379 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11983.22552 HOMO: -6.41644 LUMO: 1.78235 factor:1 | 1 (-3.67604) | -1 | -1 |
| G: -5715.18379 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.38062 HOMO: -6.59876 LUMO: 1.83677 factor:1 | 1 (-1.83114) | -1 | -1 |
| G: -5715.18379 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.34153 HOMO: -6.35658 LUMO: 1.59731 factor:1 | 1 (-2.79205) | -1 | -1 |
| G: -5715.18379 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.32330 HOMO: -6.60692 LUMO: 1.66534 factor:1 | 1 (-2.77382) | -1 | -1 |
| G: -5715.18379 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.35693 HOMO: -6.83006 LUMO: 2.11705 factor:1 | 1 (-2.80745) | -1 | -1 |
| G: -5715.18379 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.39307 HOMO: -6.89264 LUMO: 1.30070 factor:1 | 1 (-2.84359) | -1 | -1 |
| G: -5715.18379 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.35185 HOMO: -6.90081 LUMO: 2.05174 factor:1 | 1 (-2.80236) | -1 | -1 |
| G: -5715.18379 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.45634 HOMO: -6.74842 LUMO: 1.96194 factor:1 | 1 (-2.90686) | -1 | -1 |
| G: -5715.18379 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.61191 HOMO: -6.58516 LUMO: 1.30887 factor:1 | 1 (-2.06243) | -1 | -1 |
| G: -5715.18379 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.80185 HOMO: -7.00965 LUMO: 2.08167 factor:1 | 1 (-2.25237) | -1 | -1 |
| G: -5715.18379 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11983.40533 HOMO: -6.86815 LUMO: 2.29664 factor:1 | 1 (-3.85585) | -1 | -1 |
| G: -5715.18379 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11983.02438 HOMO: -6.39740 LUMO: 2.02725 factor:1 | 1 (-3.47489) | -1 | -1 |
| G: -5715.18379 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.27571 HOMO: -5.95929 LUMO: 1.62724 factor:1 | 1 (-2.72623) | -1 | -1 |
| G: -5715.18379 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.79009 HOMO: -6.71849 LUMO: 1.34696 factor:1 | 1 (-3.24060) | -1 | -1 |
| G: -5715.18379 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.42658 HOMO: -7.26816 LUMO: 1.74153 factor:1 | 1 (-1.87710) | 1 | 1 |
| G: -5715.18379 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.41155 HOMO: -6.90897 LUMO: 1.71432 factor:1 | 1 (-2.86207) | -1 | -1 |
| G: -5715.18379 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.02112 HOMO: -6.70489 LUMO: 1.91568 factor:1 | 1 (-2.47164) | -1 | -1 |
| G: -5715.18379 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.58537 HOMO: -6.83278 LUMO: 1.61908 factor:1 | 1 (-3.03589) | -1 | -1 |
| G: -5715.18379 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.63074 HOMO: -7.17292 LUMO: 1.95378 factor:1 | 1 (-2.08126) | 1 | -1 |
| G: -5715.18379 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.29485 HOMO: -6.53345 LUMO: 1.74153 factor:1 | 1 (-1.74537) | -1 | -1 |
| G: -5715.18379 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.23688 HOMO: -6.53073 LUMO: 1.51023 factor:1 | 1 (-2.68740) | -1 | -1 |
| G: -5715.18379 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.54434 HOMO: -6.93346 LUMO: 2.22861 factor:1 | 1 (-2.99486) | -1 | -1 |
| G: -5715.18379 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.89393 HOMO: -6.47903 LUMO: 2.05446 factor:1 | 1 (-2.34445) | -1 | -1 |
| G: -5715.18379 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.71417 HOMO: -6.88992 LUMO: 1.57010 factor:1 | 1 (-2.16469) | -1 | -1 |
| G: -5715.18379 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.29625 HOMO: -6.07358 LUMO: 1.95922 factor:1 | 1 (-2.74677) | -1 | -1 |
| G: -5715.18379 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.62412 HOMO: -6.75114 LUMO: 2.18780 factor:1 | 1 (-3.07464) | -1 | -1 |
| G: -5715.18379 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11983.12479 HOMO: -6.96339 LUMO: 1.70071 factor:1 | 1 (-3.57530) | -1 | -1 |
| G: -5715.18379 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.41756 HOMO: -7.14843 LUMO: 1.82588 factor:1 | 1 (-2.86808) | 1 | -1 |
| G: -5715.18379 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.85747 HOMO: -6.96339 LUMO: 2.29392 factor:1 | 1 (-2.30799) | -1 | -1 |
| G: -5715.18379 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.29012 HOMO: -6.81645 LUMO: 2.39732 factor:1 | 1 (-0.74064) | -1 | -1 |
| G: -5715.18379 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.22704 HOMO: -6.48447 LUMO: 1.24084 factor:1 | 1 (-1.67755) | -1 | -1 |
| G: -5715.18379 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.16821 HOMO: -7.14843 LUMO: 2.01092 factor:1 | 1 (-1.61872) | 1 | -1 |
| G: -5715.18379 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.04145 HOMO: -7.20013 LUMO: -0.34286 factor:1 | 1 (-1.49197) | 1 | -1 |
| G: -5715.18379 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.92634 HOMO: -6.97700 LUMO: -0.15238 factor:1 | 1 (-2.37686) | -1 | -1 |
| G: -5715.18379 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.04137 HOMO: -7.07768 LUMO: -0.26123 factor:1 | 1 (-1.49189) | 1 | -1 |
| G: -5715.18379 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.67475 HOMO: -6.99333 LUMO: -0.41361 factor:1 | 1 (-2.12526) | -1 | -1 |
| G: -5715.18379 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.10121 HOMO: -6.84638 LUMO: -0.40273 factor:1 | 1 (-1.55173) | -1 | -1 |
| G: -5715.18379 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.79302 HOMO: -6.83822 LUMO: -0.26939 factor:1 | 1 (-3.24354) | -1 | -1 |
| G: -5715.18379 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.07440 HOMO: -6.75931 LUMO: -0.93879 factor:1 | 1 (-2.52492) | -1 | -1 |
| G: -5715.18379 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.89482 HOMO: -6.79468 LUMO: -0.39729 factor:1 | 1 (-3.34534) | -1 | -1 |
| G: -5715.18379 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.09742 HOMO: -6.93890 LUMO: 0.43266 factor:1 | 1 (-2.54794) | -1 | -1 |
| G: -5715.18379 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.89589 HOMO: -7.08040 LUMO: -0.85716 factor:1 | 1 (-2.34641) | 1 | 1 |
| G: -5715.18379 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11983.48033 HOMO: -6.70216 LUMO: -1.41499 factor:1 | 1 (-3.93085) | -1 | -1 |
| G: -5715.18379 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.83365 HOMO: -6.63686 LUMO: -0.52790 factor:1 | 1 (-3.28417) | -1 | -1 |
| G: -5715.18379 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.63613 HOMO: -6.75114 LUMO: -0.13334 factor:1 | 1 (-2.08665) | -1 | -1 |
| G: -5715.18379 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.91453 HOMO: -6.94435 LUMO: -0.24490 factor:1 | 1 (-2.36505) | -1 | -1 |
| G: -5715.18379 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.92672 HOMO: -6.74298 LUMO: -0.84627 factor:1 | 1 (-2.37724) | -1 | -1 |
| G: -5715.18379 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.32521 HOMO: -7.15932 LUMO: 0.22041 factor:1 | 1 (-1.77573) | 1 | 1 |
| G: -5715.18379 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.56914 HOMO: -6.90081 LUMO: -1.16737 factor:1 | 1 (-2.01966) | -1 | -1 |
| G: -5715.18379 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.91902 HOMO: -7.04775 LUMO: -0.84355 factor:1 | 1 (-2.36954) | -1 | -1 |
| G: -5715.18379 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.87875 HOMO: -7.17020 LUMO: -1.31159 factor:1 | 1 (-2.32927) | 1 | 1 |
| G: -5715.18379 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.09268 HOMO: -7.14571 LUMO: -0.46259 factor:1 | 1 (-2.54320) | 1 | 1 |
| G: -5715.18379 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.23032 HOMO: -7.45048 LUMO: -0.91158 factor:1 | 1 (-2.68084) | 1 | 1 |
| G: -5715.18379 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.71635 HOMO: -6.87360 LUMO: -0.82995 factor:1 | 1 (-2.16687) | -1 | -1 |
| G: -5715.18379 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.72909 HOMO: -7.43415 LUMO: -0.65307 factor:1 | 1 (-2.17960) | 1 | 1 |
| G: -5715.18379 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11983.29309 HOMO: -7.47225 LUMO: -0.77280 factor:1 | 1 (-3.74361) | 1 | 1 |
| G: -5715.18379 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11983.60343 HOMO: -6.86271 LUMO: -0.83811 factor:1 | 1 (-4.05395) | -1 | -1 |
| G: -5715.18379 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11983.73846 HOMO: -7.53483 LUMO: -0.66124 factor:1 | 1 (-4.18898) | 1 | 1 |
| G: -5715.18379 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11983.19502 HOMO: -7.45864 LUMO: -1.08301 factor:1 | 1 (-3.64554) | 1 | 1 |
| G: -5715.18379 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11983.17611 HOMO: -7.24639 LUMO: -1.19186 factor:1 | 1 (-3.62662) | 1 | 1 |
| G: -5715.18379 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.08515 HOMO: -7.54844 LUMO: -0.96873 factor:1 | 1 (-2.53567) | 1 | 1 |
| G: -5715.18379 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.48301 HOMO: -7.12666 LUMO: -0.01633 factor:1 | 1 (-1.93353) | 1 | 1 |
| G: -5715.18379 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.40886 HOMO: -6.77291 LUMO: -0.70477 factor:1 | 1 (-1.85938) | -1 | -1 |
| G: -5715.18379 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.23591 HOMO: -6.76475 LUMO: -1.15921 factor:1 | 1 (-1.68643) | -1 | -1 |
| G: -5715.18379 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.26175 HOMO: -5.37697 LUMO: -0.56600 factor:1 | 1 (-2.71227) | -1 | -1 |
| G: -5715.18379 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.80111 HOMO: -6.62053 LUMO: -1.75513 factor:1 | 1 (-2.25163) | -1 | -1 |
| G: -5715.18379 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.34771 HOMO: -6.60420 LUMO: -1.74697 factor:1 | 1 (-2.79823) | -1 | -1 |
| G: -5715.18379 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.25062 HOMO: -6.84366 LUMO: -0.94968 factor:1 | 1 (-2.70114) | -1 | -1 |
| G: -5715.18379 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11983.29404 HOMO: -6.96884 LUMO: -2.11977 factor:1 | 1 (-3.74456) | -1 | -1 |
| G: -5715.18379 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.20131 HOMO: -6.80829 LUMO: 0.56055 factor:1 | 1 (-2.65183) | -1 | -1 |
| G: -5715.18379 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11983.13143 HOMO: -7.02326 LUMO: 0.11429 factor:1 | 1 (-3.58194) | -1 | -1 |
| G: -5715.18379 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.85327 HOMO: -7.40966 LUMO: 0.18232 factor:1 | 1 (-3.30379) | 1 | 1 |
| G: -5715.18379 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.26847 HOMO: -6.34570 LUMO: 0.41089 factor:1 | 1 (-2.71899) | -1 | -1 |
| G: -5715.18379 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.24063 HOMO: -6.78924 LUMO: 0.49525 factor:1 | 1 (-2.69115) | -1 | -1 |
| G: -5715.18379 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.58242 HOMO: -6.87632 LUMO: 0.44082 factor:1 | 1 (-2.03294) | -1 | -1 |
| G: -5715.18379 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.69906 HOMO: -6.69944 LUMO: 1.20546 factor:1 | 1 (-3.14958) | -1 | -1 |
| G: -5715.18379 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.65072 HOMO: -6.83006 LUMO: 1.28982 factor:1 | 1 (-2.10124) | -1 | -1 |
| G: -5715.18379 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.96166 HOMO: -7.78246 LUMO: 0.20681 factor:1 | 1 (-2.41218) | 1 | 1 |
| G: -5715.18379 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.07312 HOMO: -6.55794 LUMO: -1.65173 factor:1 | 1 (-2.52364) | -1 | -1 |
| G: -5715.18379 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.25854 HOMO: -6.77564 LUMO: -1.14560 factor:1 | 1 (-2.70906) | -1 | -1 |
| G: -5715.18379 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.90917 HOMO: -7.46680 LUMO: -1.18097 factor:1 | 1 (-2.35969) | 1 | 1 |
| G: -5715.18379 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.21843 HOMO: -6.88176 LUMO: -1.24900 factor:1 | 1 (-2.66895) | -1 | -1 |
| G: -5715.18379 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11983.17673 HOMO: -7.28177 LUMO: -0.42178 factor:1 | 1 (-3.62725) | 1 | 1 |
| G: -5715.18379 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11983.11730 HOMO: -7.71715 LUMO: 0.19592 factor:1 | 1 (-3.56782) | 1 | 1 |
| G: -5715.18379 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.95919 HOMO: -7.02326 LUMO: -1.40683 factor:1 | 1 (-2.40970) | -1 | -1 |
| G: -5715.18379 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.03582 HOMO: -7.27088 LUMO: -1.07485 factor:1 | 1 (-1.48634) | 1 | 1 |
| G: -5715.18379 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.93909 HOMO: -7.17020 LUMO: -0.49525 factor:1 | 1 (-1.38960) | 1 | 1 |
| G: -5715.18379 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.57990 HOMO: -7.15932 LUMO: 0.02721 factor:1 | 1 (-1.03041) | 1 | 1 |
| G: -5715.18379 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.88252 HOMO: -7.00693 LUMO: -0.83267 factor:1 | 1 (-3.33304) | -1 | -1 |
| G: -5715.18379 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.02433 HOMO: -6.86543 LUMO: -0.10340 factor:1 | 1 (-2.47485) | -1 | -1 |
| G: -5715.18379 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.68546 HOMO: -7.11850 LUMO: -0.08980 factor:1 | 1 (-3.13598) | 1 | 1 |
| G: -5715.18379 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.61610 HOMO: -6.87087 LUMO: -0.88981 factor:1 | 1 (-2.06662) | -1 | -1 |
| G: -5715.18379 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11979.46687 HOMO: -7.08857 LUMO: -1.27077 factor:1 | -1 (0.08261) | 1 | 1 |
| G: -5715.18379 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.04079 HOMO: -6.79468 LUMO: -0.81906 factor:1 | 1 (-2.49131) | -1 | -1 |
| G: -5715.18379 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.54377 HOMO: -6.86815 LUMO: -0.89798 factor:1 | 1 (-2.99429) | -1 | -1 |
| G: -5715.18379 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.65172 HOMO: -6.78652 LUMO: -2.00548 factor:1 | 1 (-2.10224) | -1 | -1 |
| G: -5715.18379 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.30423 HOMO: -6.75114 LUMO: -0.08436 factor:1 | 1 (-1.75475) | -1 | -1 |
| G: -5715.18379 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.32588 HOMO: -6.55794 LUMO: 0.52790 factor:1 | 1 (-0.77640) | -1 | -1 |
| G: -5715.18379 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.16639 HOMO: -7.17836 LUMO: 0.28300 factor:1 | 1 (-0.61691) | 1 | -1 |
| G: -5715.18379 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.31247 HOMO: -7.35796 LUMO: -0.77552 factor:1 | 1 (-2.76299) | 1 | 1 |
| G: -5715.18379 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.33857 HOMO: -7.23551 LUMO: -1.17553 factor:1 | 1 (-2.78909) | 1 | 1 |
| G: -5715.18379 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.35000 HOMO: -7.07496 LUMO: -1.14288 factor:1 | 1 (-2.80051) | 1 | 1 |
| G: -5715.18379 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.72596 HOMO: -6.70489 LUMO: -0.83539 factor:1 | 1 (-2.17648) | -1 | -1 |
| G: -5715.18379 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.46309 HOMO: -6.59604 LUMO: -0.89798 factor:1 | 1 (-2.91360) | -1 | -1 |
| G: -5715.18379 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.82185 HOMO: -6.94162 LUMO: -1.22451 factor:1 | 1 (-2.27237) | -1 | -1 |
| G: -5715.18379 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.52184 HOMO: -6.68040 LUMO: 0.22041 factor:1 | 1 (-1.97236) | -1 | -1 |
| G: -5715.18379 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.86566 HOMO: -6.88176 LUMO: 0.11157 factor:1 | 1 (-2.31618) | -1 | -1 |
| G: -5715.18379 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.25797 HOMO: -6.91713 LUMO: 1.27621 factor:1 | 1 (-2.70849) | -1 | -1 |
| G: -5715.18379 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.37938 HOMO: -6.77836 LUMO: 1.01226 factor:1 | 1 (-2.82990) | -1 | -1 |
| G: -5715.18379 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.56861 HOMO: -7.14571 LUMO: 1.48574 factor:1 | 1 (-3.01913) | 1 | 1 |
| G: -5715.18379 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.32651 HOMO: -6.96884 LUMO: 1.48574 factor:1 | 1 (-2.77703) | -1 | -1 |
| G: -5715.18379 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.61240 HOMO: -7.24367 LUMO: 1.28438 factor:1 | 1 (-2.06292) | 1 | 1 |
| G: -5715.18379 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.06463 HOMO: -7.10489 LUMO: 1.29526 factor:1 | 1 (-2.51515) | 1 | 1 |
| G: -5715.18379 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.16136 HOMO: -7.07224 LUMO: 1.29254 factor:1 | 1 (-0.61188) | 1 | 1 |
| G: -5715.18379 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.28985 HOMO: -7.12938 LUMO: 0.49253 factor:1 | 1 (-0.74037) | 1 | 1 |
| G: -5715.18379 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.12265 HOMO: -7.33619 LUMO: 1.45581 factor:1 | 1 (-1.57317) | 1 | 1 |
| G: -5715.18379 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.48944 HOMO: -6.87904 LUMO: -0.14422 factor:1 | 1 (-1.93995) | -1 | -1 |
| G: -5715.18379 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.03911 HOMO: -6.81917 LUMO: 0.50341 factor:1 | 1 (-1.48963) | -1 | -1 |
| G: -5715.18379 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.98430 HOMO: -7.27905 LUMO: 0.13606 factor:1 | 1 (-2.43482) | 1 | -1 |
| G: -5715.18379 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.18170 HOMO: -6.87904 LUMO: -0.09796 factor:1 | 1 (-1.63222) | -1 | -1 |
| G: -5715.18379 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.11811 HOMO: -7.33891 LUMO: 0.03810 factor:1 | 1 (-1.56863) | 1 | 1 |
| G: -5715.18379 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.63078 HOMO: -6.98516 LUMO: 0.98233 factor:1 | 1 (-1.08130) | -1 | -1 |
| G: -5715.18379 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.43010 HOMO: -6.94162 LUMO: 0.86804 factor:1 | 1 (-0.88061) | -1 | -1 |
| G: -5715.18379 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.26617 HOMO: -7.37701 LUMO: 0.05442 factor:1 | 1 (-0.71669) | 1 | 1 |
| G: -5715.18379 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.46623 HOMO: -7.04775 LUMO: 0.43266 factor:1 | 1 (-0.91675) | -1 | -1 |
| G: -5715.18379 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.05082 HOMO: -7.47497 LUMO: 0.31837 factor:1 | 1 (-1.50133) | 1 | 1 |
| G: -5715.18379 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11979.69694 HOMO: -6.62053 LUMO: 0.13061 factor:1 | 1 (-0.14746) | -1 | -1 |
| G: -5715.18379 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.25292 HOMO: -6.44366 LUMO: -0.04354 factor:1 | 1 (-0.70344) | -1 | -1 |
| G: -5715.18379 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.23480 HOMO: -6.40284 LUMO: 0.68301 factor:1 | 1 (-0.68532) | -1 | -1 |
| G: -5715.18379 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.40894 HOMO: -6.73754 LUMO: 0.36735 factor:1 | 1 (-2.85945) | -1 | -1 |
| G: -5715.18379 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.56687 HOMO: -6.85455 LUMO: 0.23946 factor:1 | 1 (-3.01739) | -1 | -1 |
| G: -5715.18379 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.39408 HOMO: -6.93346 LUMO: 0.24762 factor:1 | 1 (-2.84460) | -1 | -1 |
| G: -5715.18379 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.55755 HOMO: -6.85455 LUMO: 0.17687 factor:1 | 1 (-2.00806) | -1 | -1 |
| G: -5715.18379 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.93147 HOMO: -6.62325 LUMO: 0.69933 factor:1 | 1 (-1.38198) | -1 | -1 |
| G: -5715.18379 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.52809 HOMO: -6.43005 LUMO: 0.50069 factor:1 | 1 (-2.97861) | -1 | -1 |
| G: -5715.18379 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.95723 HOMO: -6.56883 LUMO: 0.22858 factor:1 | 1 (-2.40775) | -1 | -1 |
| G: -5715.18379 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.41474 HOMO: -6.78380 LUMO: 0.54967 factor:1 | 1 (-1.86526) | -1 | -1 |
| G: -5715.18379 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.07043 HOMO: -7.35524 LUMO: 0.00272 factor:1 | 1 (-2.52094) | 1 | 1 |
| G: -5715.18379 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.31969 HOMO: -7.27360 LUMO: 0.08436 factor:1 | 1 (-1.77021) | 1 | 1 |
| G: -5715.18379 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.07575 HOMO: -7.44504 LUMO: -0.96056 factor:1 | 1 (-0.52627) | 1 | 1 |
| G: -5715.18379 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11979.40126 HOMO: -7.27360 LUMO: 0.29933 factor:1 | -1 (0.14822) | 1 | 1 |
| G: -5715.18379 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11979.46828 HOMO: -7.09129 LUMO: 0.41089 factor:1 | -1 (0.08120) | 1 | 1 |
| G: -5715.18379 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11978.90525 HOMO: -6.93618 LUMO: 0.36463 factor:1 | -1 (0.64423) | -1 | -1 |
| G: -5715.18379 HOMO: -7.26000 LUMO: -3.02863 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.16764 HOMO: -7.65728 LUMO: 0.20136 factor:1 | 1 (-0.61816) | 1 | 1 |
| G: -5715.18379 HOMO: -7.26000 LUMO: -3.02863 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.43834 HOMO: -6.90353 LUMO: -0.92791 factor:1 | 1 (-0.88886) | -1 | -1 |
| G: -5715.18379 HOMO: -7.26000 LUMO: -3.02863 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.33148 HOMO: -6.82462 LUMO: -1.18370 factor:1 | 1 (-0.78200) | -1 | -1 |
| G: -5715.18379 HOMO: -7.26000 LUMO: -3.02863 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.22763 HOMO: -7.09129 LUMO: -0.13334 factor:1 | 1 (-2.67814) | 1 | 1 |
| G: -5715.18379 HOMO: -7.26000 LUMO: -3.02863 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.38874 HOMO: -7.40966 LUMO: -1.06941 factor:1 | 1 (-2.83926) | 1 | 1 |
| G: -5715.18379 HOMO: -7.26000 LUMO: -3.02863 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.83437 HOMO: -7.24367 LUMO: -1.00954 factor:1 | 1 (-2.28489) | 1 | 1 |
| G: -5715.18379 HOMO: -7.26000 LUMO: -3.02863 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.50143 HOMO: -7.51851 LUMO: 0.09796 factor:1 | 1 (-2.95195) | 1 | 1 |
| G: -5715.18379 HOMO: -7.26000 LUMO: -3.02863 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.39367 HOMO: -7.48857 LUMO: -0.07619 factor:1 | 1 (-2.84419) | 1 | 1 |
| G: -5715.18379 HOMO: -7.26000 LUMO: -3.02863 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.45141 HOMO: -6.53345 LUMO: 1.09390 factor:1 | 1 (-2.90193) | -1 | -1 |
| G: -5715.18379 HOMO: -7.26000 LUMO: -3.02863 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.87135 HOMO: -7.21918 LUMO: 0.08436 factor:1 | 1 (-2.32187) | 1 | 1 |
| G: -5715.18379 HOMO: -7.26000 LUMO: -3.02863 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.34711 HOMO: -7.38789 LUMO: 1.02587 factor:1 | 1 (-2.79763) | 1 | -1 |
| G: -5715.18379 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.46766 HOMO: -6.83550 LUMO: -0.67484 factor:1 | 1 (-2.91818) | -1 | -1 |
| G: -5715.18379 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.65635 HOMO: -7.04231 LUMO: 0.54151 factor:1 | 1 (-2.10687) | -1 | -1 |
| G: -5715.18379 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.18606 HOMO: -6.79740 LUMO: 1.91296 factor:1 | 1 (-1.63657) | 1 | 1 |
| G: -5715.18379 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.98808 HOMO: -7.35796 LUMO: -1.04220 factor:1 | 1 (-2.43860) | -1 | -1 |
| G: -5715.18379 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.48935 HOMO: -6.62597 LUMO: -0.44082 factor:1 | 1 (-1.93987) | -1 | -1 |
| G: -5715.18379 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.18100 HOMO: -6.45182 LUMO: -0.20409 factor:1 | 1 (-0.63152) | -1 | -1 |
| G: -5715.18379 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.29048 HOMO: -6.51168 LUMO: -0.23130 factor:1 | 1 (-2.74100) | -1 | -1 |
| G: -5715.18379 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.40453 HOMO: -7.14027 LUMO: 0.49797 factor:1 | 1 (-2.85505) | -1 | -1 |
| G: -5715.18379 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.37176 HOMO: -7.55660 LUMO: 0.24762 factor:1 | 1 (-2.82228) | -1 | -1 |
| G: -5715.18379 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.99140 HOMO: -6.88992 LUMO: -0.64763 factor:1 | 1 (-2.44192) | -1 | -1 |
| G: -5715.18379 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.49480 HOMO: -6.72665 LUMO: -0.45987 factor:1 | 1 (-1.94531) | -1 | -1 |
| G: -5715.18379 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.11889 HOMO: -6.72121 LUMO: -0.58232 factor:1 | 1 (-2.56941) | -1 | -1 |
| G: -5715.18379 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.13423 HOMO: -7.26816 LUMO: 0.32926 factor:1 | 1 (-0.58475) | -1 | -1 |
| G: -5715.18379 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.22533 HOMO: -6.57155 LUMO: -0.53606 factor:1 | 1 (-0.67585) | -1 | -1 |
| G: -5715.18379 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.04311 HOMO: -6.50896 LUMO: -0.43810 factor:1 | 1 (-2.49362) | -1 | -1 |
| G: -5715.18379 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.12418 HOMO: -6.73210 LUMO: -0.51430 factor:1 | 1 (-1.57470) | -1 | -1 |
| G: -5715.18379 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.91500 HOMO: -6.77019 LUMO: -0.62858 factor:1 | 1 (-1.36552) | -1 | -1 |
| G: -5715.18379 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.18627 HOMO: -6.82462 LUMO: -0.67484 factor:1 | 1 (-1.63679) | -1 | -1 |
| G: -5715.18379 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.15142 HOMO: -6.79740 LUMO: -0.55511 factor:1 | 1 (-0.60194) | -1 | -1 |
| G: -5715.18379 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.19662 HOMO: -6.79740 LUMO: -0.67756 factor:1 | 1 (-0.64714) | -1 | -1 |
| G: -5715.18379 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.57109 HOMO: -6.75114 LUMO: -0.55239 factor:1 | 1 (-3.02161) | -1 | -1 |
| G: -5715.18379 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.18259 HOMO: -6.49536 LUMO: -0.25307 factor:1 | 1 (-2.63311) | -1 | -1 |
| G: -5715.18379 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11983.45802 HOMO: -6.48992 LUMO: -0.25034 factor:1 | 1 (-3.90853) | -1 | -1 |
| G: -5715.18379 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.61691 HOMO: -6.52801 LUMO: -0.28028 factor:1 | 1 (-3.06743) | -1 | -1 |
| G: -5715.18379 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11983.37848 HOMO: -7.22462 LUMO: 0.52518 factor:1 | 1 (-3.82900) | -1 | -1 |
| G: -5715.18379 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.46173 HOMO: -6.59332 LUMO: -0.27211 factor:1 | 1 (-2.91224) | -1 | -1 |
| G: -5715.18379 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.56475 HOMO: -6.57427 LUMO: -0.16871 factor:1 | 1 (-3.01527) | -1 | -1 |
| G: -5715.18379 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11983.19192 HOMO: -6.71033 LUMO: 1.59187 factor:1 | 1 (-3.64243) | 1 | 1 |
| G: -5715.18379 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11983.08122 HOMO: -6.72121 LUMO: 2.00004 factor:1 | 1 (-3.53174) | 1 | 1 |
| G: -5715.18379 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.33459 HOMO: -6.61509 LUMO: 1.55921 factor:1 | 1 (-2.78511) | -1 | -1 |
| G: -5715.18379 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.58167 HOMO: -6.55250 LUMO: 1.73064 factor:1 | 1 (-3.03219) | -1 | -1 |
| G: -5715.18379 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.28174 HOMO: -6.66135 LUMO: 2.02181 factor:1 | 1 (-0.73226) | 1 | 1 |
| G: -5715.18379 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.05935 HOMO: -6.84911 LUMO: 1.98099 factor:1 | 1 (-2.50987) | 1 | 1 |
| G: -5715.18379 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.72681 HOMO: -6.66679 LUMO: 1.98371 factor:1 | 1 (-1.17733) | 1 | 1 |
| G: -5715.18379 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.99193 HOMO: -6.67495 LUMO: 2.04085 factor:1 | 1 (-1.44245) | 1 | 1 |
| G: -5715.18379 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.20847 HOMO: -6.89809 LUMO: 1.95106 factor:1 | 1 (-2.65899) | 1 | 1 |
| G: -5715.18379 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.99826 HOMO: -6.50352 LUMO: 1.88847 factor:1 | 1 (-2.44878) | -1 | -1 |
| G: -5715.18379 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.29489 HOMO: -6.93618 LUMO: 2.00004 factor:1 | 1 (-2.74541) | 1 | 1 |
| G: -5715.18379 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11983.30073 HOMO: -6.50896 LUMO: 1.73609 factor:1 | 1 (-3.75125) | -1 | -1 |
| G: -5715.18379 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11983.18530 HOMO: -6.69672 LUMO: 2.37283 factor:1 | 1 (-3.63582) | 1 | 1 |
| G: -5715.18379 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.47351 HOMO: -6.65591 LUMO: 2.20684 factor:1 | 1 (-2.92403) | 1 | 1 |
| G: -5715.18379 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.40455 HOMO: -6.23957 LUMO: 1.78507 factor:1 | 1 (-2.85507) | -1 | -1 |
| G: -5715.18379 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.56405 HOMO: -6.35114 LUMO: 1.92112 factor:1 | 1 (-2.01457) | -1 | -1 |
| G: -5715.18379 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.20833 HOMO: -6.53617 LUMO: 1.75241 factor:1 | 1 (-2.65885) | -1 | -1 |
| G: -5715.18379 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.89188 HOMO: -6.60420 LUMO: 1.78779 factor:1 | 1 (-3.34240) | 1 | 1 |
| G: -5715.18379 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.49752 HOMO: -7.40422 LUMO: -0.97145 factor:1 | 1 (-1.94804) | -1 | -1 |
| G: -5715.18379 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.15065 HOMO: -6.80013 LUMO: -0.69117 factor:1 | 1 (-2.60116) | -1 | -1 |
| G: -5715.18379 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11983.10680 HOMO: -6.68040 LUMO: -0.47076 factor:1 | 1 (-3.55732) | -1 | -1 |
| G: -5715.18379 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.95298 HOMO: -7.20285 LUMO: -0.66124 factor:1 | 1 (-2.40350) | -1 | -1 |
| G: -5715.18379 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11983.51521 HOMO: -6.82734 LUMO: -0.60137 factor:1 | 1 (-3.96573) | -1 | -1 |
| G: -5715.18379 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11983.59181 HOMO: -7.18653 LUMO: 0.59321 factor:1 | 1 (-4.04233) | -1 | -1 |
| G: -5715.18379 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.14311 HOMO: -7.29265 LUMO: 0.48164 factor:1 | 1 (-2.59363) | -1 | -1 |
| G: -5715.18379 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.25244 HOMO: -6.63414 LUMO: -0.25034 factor:1 | 1 (-2.70296) | -1 | -1 |
| G: -5715.18379 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.28594 HOMO: -7.20285 LUMO: 0.53879 factor:1 | 1 (-2.73646) | -1 | -1 |
| G: -5715.18379 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.28948 HOMO: -6.46815 LUMO: -0.21769 factor:1 | 1 (-2.74000) | -1 | -1 |
| G: -5715.18379 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.67189 HOMO: -6.57971 LUMO: -0.18776 factor:1 | 1 (-2.12241) | -1 | -1 |
| G: -5715.18379 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.77379 HOMO: -6.90897 LUMO: 1.91296 factor:1 | 1 (-2.22431) | 1 | 1 |
| G: -5715.18379 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.88240 HOMO: -6.67495 LUMO: 2.04358 factor:1 | 1 (-1.33292) | 1 | 1 |
| G: -5715.18379 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11983.45706 HOMO: -6.94162 LUMO: 1.73881 factor:1 | 1 (-3.90758) | 1 | 1 |
| G: -5715.18379 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11983.04201 HOMO: -6.73482 LUMO: 1.95922 factor:1 | 1 (-3.49253) | 1 | 1 |
| G: -5715.18379 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11983.24778 HOMO: -6.70489 LUMO: 2.04358 factor:1 | 1 (-3.69830) | 1 | 1 |
| G: -5715.18379 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.95459 HOMO: -7.04231 LUMO: 1.79323 factor:1 | 1 (-2.40511) | 1 | 1 |
| G: -5715.18379 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.20665 HOMO: -6.68584 LUMO: 1.60275 factor:1 | 1 (-2.65716) | 1 | 1 |
| G: -5715.18379 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.34959 HOMO: -6.40556 LUMO: 1.45581 factor:1 | 1 (-2.80011) | -1 | -1 |
| G: -5715.18379 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11983.02487 HOMO: -6.94979 LUMO: 2.16603 factor:1 | 1 (-3.47538) | 1 | 1 |
| G: -5715.18379 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.05598 HOMO: -6.84911 LUMO: 1.89935 factor:1 | 1 (-2.50650) | 1 | 1 |
| G: -5715.18379 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.32481 HOMO: -6.22052 LUMO: 1.57282 factor:1 | 1 (-1.77533) | -1 | -1 |
| G: -5715.18379 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.42785 HOMO: -6.51168 LUMO: 2.10072 factor:1 | 1 (-2.87837) | -1 | -1 |
| G: -5715.18379 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.87505 HOMO: -7.03686 LUMO: 2.12249 factor:1 | 1 (-2.32557) | 1 | 1 |
| G: -5715.18379 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.46273 HOMO: -6.84094 LUMO: 1.63268 factor:1 | 1 (-2.91325) | 1 | 1 |
| G: -5715.18379 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.42797 HOMO: -6.75387 LUMO: 1.72248 factor:1 | 1 (-1.87848) | 1 | 1 |
| G: -5715.18379 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.55482 HOMO: -6.86271 LUMO: 1.68711 factor:1 | 1 (-2.00534) | 1 | 1 |
| G: -5715.18379 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.29520 HOMO: -6.84094 LUMO: 2.02997 factor:1 | 1 (-1.74572) | 1 | 1 |
| G: -5715.18379 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.83974 HOMO: -6.80557 LUMO: 2.02725 factor:1 | 1 (-1.29026) | 1 | 1 |
| G: -5715.18379 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.32447 HOMO: -6.38651 LUMO: 1.53472 factor:1 | 1 (-2.77499) | -1 | -1 |
| G: -5715.18379 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.20213 HOMO: -7.51306 LUMO: 0.28572 factor:1 | 1 (-2.65265) | -1 | -1 |
| G: -5715.18379 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.17290 HOMO: -6.97972 LUMO: -0.74287 factor:1 | 1 (-2.62342) | -1 | -1 |
| G: -5715.18379 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.21734 HOMO: -6.83822 LUMO: -0.65852 factor:1 | 1 (-2.66786) | -1 | -1 |
| G: -5715.18379 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.54250 HOMO: -6.71305 LUMO: -0.49525 factor:1 | 1 (-1.99302) | -1 | -1 |
| G: -5715.18379 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.42268 HOMO: -6.60692 LUMO: -0.22313 factor:1 | 1 (-2.87320) | -1 | -1 |
| G: -5715.18379 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.76345 HOMO: -7.20013 LUMO: 0.55239 factor:1 | 1 (-2.21397) | -1 | -1 |
| G: -5715.18379 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.59553 HOMO: -6.60420 LUMO: -0.28028 factor:1 | 1 (-2.04605) | -1 | -1 |
| G: -5715.18379 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.53087 HOMO: -6.69128 LUMO: -0.30477 factor:1 | 1 (-2.98139) | -1 | -1 |
| G: -5715.18379 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.13609 HOMO: -6.65591 LUMO: -0.25579 factor:1 | 1 (-2.58661) | -1 | -1 |
| G: -5715.18379 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.58280 HOMO: -6.69128 LUMO: 1.70888 factor:1 | 1 (-2.03332) | 1 | 1 |
| G: -5715.18379 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.60453 HOMO: -6.50080 LUMO: 1.87759 factor:1 | 1 (-3.05505) | -1 | -1 |
| G: -5715.18379 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.10425 HOMO: -6.85727 LUMO: 1.99187 factor:1 | 1 (-2.55477) | 1 | 1 |
| G: -5715.18379 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11983.08106 HOMO: -6.58788 LUMO: 1.79051 factor:1 | 1 (-3.53158) | 1 | 1 |
| G: -5715.18379 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.35370 HOMO: -6.64230 LUMO: 2.16058 factor:1 | 1 (-2.80421) | 1 | 1 |
| G: -5715.18379 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.88289 HOMO: -6.58788 LUMO: 2.10616 factor:1 | 1 (-2.33340) | 1 | 1 |
| G: -5715.18379 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.07453 HOMO: -7.01782 LUMO: 2.13609 factor:1 | 1 (-2.52505) | 1 | 1 |
| G: -5715.18379 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.91799 HOMO: -6.31304 LUMO: 2.31841 factor:1 | 1 (-2.36851) | -1 | -1 |
| G: -5715.18379 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.76337 HOMO: -6.94979 LUMO: 2.07895 factor:1 | 1 (-2.21389) | 1 | 1 |
| G: -5715.18379 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.91233 HOMO: -6.88992 LUMO: 2.28031 factor:1 | 1 (-2.36285) | 1 | 1 |
| G: -5715.18379 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.27894 HOMO: -6.66407 LUMO: 2.07623 factor:1 | 1 (-0.72946) | 1 | 1 |
| G: -5715.18379 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.28977 HOMO: -6.52529 LUMO: 1.70071 factor:1 | 1 (-0.74029) | -1 | -1 |
| G: -5715.18379 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.18808 HOMO: -6.58788 LUMO: 1.57282 factor:1 | 1 (-0.63860) | -1 | -1 |
| G: -5715.18379 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.26555 HOMO: -6.55250 LUMO: 1.95378 factor:1 | 1 (-0.71607) | -1 | -1 |
| G: -5715.18379 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.22517 HOMO: -6.24773 LUMO: 1.77962 factor:1 | 1 (-0.67569) | -1 | -1 |
| G: -5715.18379 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11979.90290 HOMO: -6.31304 LUMO: 2.18507 factor:1 | 1 (-0.35342) | -1 | -1 |
| G: -5715.18379 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.13507 HOMO: -6.18243 LUMO: 2.01636 factor:1 | 1 (-0.58559) | -1 | -1 |
| G: -5715.18379 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.10936 HOMO: -6.99877 LUMO: 2.14970 factor:1 | 1 (-0.55987) | 1 | 1 |
| G: -5715.18379 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11979.99776 HOMO: -6.72665 LUMO: 2.07079 factor:1 | 1 (-0.44828) | 1 | 1 |
| G: -5715.18379 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.34077 HOMO: -6.36202 LUMO: 2.17419 factor:1 | 1 (-2.79129) | -1 | -1 |
| G: -5715.18379 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.26774 HOMO: -6.78652 LUMO: 2.05718 factor:1 | 1 (-2.71825) | 1 | -1 |
| G: -5715.18379 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.32072 HOMO: -6.87360 LUMO: 2.34290 factor:1 | 1 (-2.77123) | 1 | 1 |
| G: -5715.18379 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.44616 HOMO: -6.62053 LUMO: 1.89391 factor:1 | 1 (-2.89668) | 1 | 1 |
| G: -5715.18379 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.31778 HOMO: -6.58788 LUMO: 1.83133 factor:1 | 1 (-2.76830) | 1 | 1 |
| G: -5715.18379 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.40401 HOMO: -7.08584 LUMO: 1.91568 factor:1 | 1 (-2.85453) | 1 | 1 |
| G: -5715.18379 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.64838 HOMO: -6.56883 LUMO: 1.81228 factor:1 | 1 (-2.09890) | 1 | 1 |
| G: -5715.18379 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.86645 HOMO: -6.66135 LUMO: 1.92384 factor:1 | 1 (-2.31697) | 1 | 1 |
| G: -5715.18379 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.26655 HOMO: -6.64502 LUMO: 2.15786 factor:1 | 1 (-1.71707) | 1 | 1 |
| G: -5715.18379 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.39353 HOMO: -6.71305 LUMO: 1.91840 factor:1 | 1 (-2.84405) | 1 | 1 |
| G: -5715.18379 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.29576 HOMO: -6.44094 LUMO: 1.74425 factor:1 | 1 (-2.74628) | -1 | -1 |
| G: -5715.18379 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.95354 HOMO: -6.51985 LUMO: 1.84221 factor:1 | 1 (-3.40406) | -1 | -1 |
| G: -5715.18379 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.15859 HOMO: -6.63414 LUMO: -0.24762 factor:1 | 1 (-2.60911) | -1 | -1 |
| G: -5715.18379 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.14616 HOMO: -6.60420 LUMO: -0.22585 factor:1 | 1 (-2.59667) | -1 | -1 |
| G: -5715.18379 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.78884 HOMO: -7.19741 LUMO: 0.58232 factor:1 | 1 (-2.23936) | -1 | -1 |
| G: -5715.18379 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.40583 HOMO: -6.77019 LUMO: -0.56872 factor:1 | 1 (-2.85635) | -1 | -1 |
| G: -5715.18379 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.32730 HOMO: -7.46136 LUMO: 0.28844 factor:1 | 1 (-2.77782) | -1 | -1 |
| G: -5715.18379 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.59857 HOMO: -6.60420 LUMO: -0.54151 factor:1 | 1 (-3.04909) | -1 | -1 |
| G: -5715.18379 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11983.22520 HOMO: -6.53890 LUMO: -0.46531 factor:1 | 1 (-3.67571) | -1 | -1 |
| G: -5715.18379 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.91112 HOMO: -6.81645 LUMO: -0.57144 factor:1 | 1 (-3.36164) | -1 | -1 |
| G: -5715.18379 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11983.03150 HOMO: -7.48041 LUMO: 0.28572 factor:1 | 1 (-3.48202) | -1 | -1 |
| G: -5715.18379 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.04445 HOMO: -6.75659 LUMO: -0.45715 factor:1 | 1 (-1.49497) | -1 | -1 |
| G: -5715.18379 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.95639 HOMO: -6.66135 LUMO: -0.41906 factor:1 | 1 (-1.40691) | -1 | -1 |
| G: -5715.18379 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.70737 HOMO: -6.55794 LUMO: -0.27483 factor:1 | 1 (-2.15789) | -1 | -1 |
| G: -5715.18379 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.02227 HOMO: -7.07496 LUMO: -0.63403 factor:1 | 1 (-1.47279) | -1 | -1 |
| G: -5715.18379 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.39964 HOMO: -7.12394 LUMO: 0.53334 factor:1 | 1 (-1.85016) | -1 | -1 |
| G: -5715.18379 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.81456 HOMO: -6.53617 LUMO: -0.25579 factor:1 | 1 (-2.26508) | -1 | -1 |
| G: -5715.18379 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.10796 HOMO: -6.50896 LUMO: -0.25034 factor:1 | 1 (-1.55848) | -1 | -1 |
| G: -5715.18379 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.63088 HOMO: -7.17564 LUMO: -0.68573 factor:1 | 1 (-2.08140) | -1 | -1 |
| G: -5715.18379 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.90197 HOMO: -6.53617 LUMO: -0.30749 factor:1 | 1 (-1.35249) | -1 | -1 |
| G: -5715.18379 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.68443 HOMO: -6.55522 LUMO: -0.30749 factor:1 | 1 (-2.13495) | -1 | -1 |
| G: -5715.18379 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.05599 HOMO: -7.05591 LUMO: -0.71022 factor:1 | 1 (-1.50650) | -1 | -1 |
| G: -5715.18379 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.88833 HOMO: -7.17564 LUMO: -0.69933 factor:1 | 1 (-2.33885) | -1 | -1 |
| G: -5715.18379 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.08829 HOMO: -6.78380 LUMO: -0.67756 factor:1 | 1 (-1.53880) | -1 | -1 |
| G: -5715.18379 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.42554 HOMO: -6.62325 LUMO: 2.02725 factor:1 | 1 (-1.87606) | 1 | 1 |
| G: -5715.18379 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.89679 HOMO: -6.63414 LUMO: 1.91296 factor:1 | 1 (-2.34731) | 1 | -1 |
| G: -5715.18379 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.76043 HOMO: -6.83278 LUMO: 1.65717 factor:1 | 1 (-2.21095) | 1 | 1 |
| G: -5715.18379 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.85233 HOMO: -6.66407 LUMO: 1.95650 factor:1 | 1 (-2.30285) | 1 | 1 |
| G: -5715.18379 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.31614 HOMO: -6.61237 LUMO: 2.11432 factor:1 | 1 (-2.76666) | 1 | 1 |
| G: -5715.18379 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.24036 HOMO: -6.62053 LUMO: 2.09256 factor:1 | 1 (-2.69088) | 1 | -1 |
| G: -5715.18379 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.20363 HOMO: -6.78652 LUMO: 2.13609 factor:1 | 1 (-2.65414) | 1 | 1 |
| G: -5715.18379 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11983.62659 HOMO: -6.94707 LUMO: 1.81772 factor:1 | 1 (-4.07711) | 1 | 1 |
| G: -5715.18379 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11983.58303 HOMO: -6.85183 LUMO: 2.12793 factor:1 | 1 (-4.03354) | 1 | 1 |
| G: -5715.18379 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11983.61824 HOMO: -6.81101 LUMO: 1.83949 factor:1 | 1 (-4.06876) | 1 | 1 |
| G: -5715.18379 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11983.25069 HOMO: -6.98788 LUMO: 2.16058 factor:1 | 1 (-3.70121) | 1 | 1 |
| G: -5715.18379 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.60108 HOMO: -6.62869 LUMO: 2.00820 factor:1 | 1 (-2.05160) | 1 | 1 |
| G: -5715.18379 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.24110 HOMO: -6.34025 LUMO: 2.25855 factor:1 | 1 (-2.69161) | -1 | -1 |
| G: -5715.18379 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11979.80709 HOMO: -6.01372 LUMO: 2.01636 factor:1 | 1 (-0.25761) | -1 | -1 |
| G: -5715.18379 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.27601 HOMO: -6.89264 LUMO: 2.27487 factor:1 | 1 (-2.72653) | 1 | 1 |
| G: -5715.18379 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.17837 HOMO: -6.53073 LUMO: 2.20684 factor:1 | 1 (-2.62889) | -1 | -1 |
| G: -5715.18379 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.84222 HOMO: -6.83278 LUMO: 1.53744 factor:1 | 1 (-3.29274) | -1 | -1 |
| G: -5715.18379 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.96844 HOMO: -6.41917 LUMO: 1.82316 factor:1 | 1 (-2.41896) | -1 | -1 |
| G: -5715.18379 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.34428 HOMO: -6.56339 LUMO: 1.63813 factor:1 | 1 (-2.79480) | -1 | -1 |
| G: -5715.18379 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.33133 HOMO: -6.88992 LUMO: 1.65173 factor:1 | 1 (-2.78185) | 1 | 1 |
| G: -5715.18379 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.69936 HOMO: -6.63141 LUMO: 1.92112 factor:1 | 1 (-3.14988) | 1 | 1 |
| G: -5715.18379 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.01410 HOMO: -6.83822 LUMO: 1.88847 factor:1 | 1 (-2.46462) | 1 | 1 |
| G: -5715.18379 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.32772 HOMO: -6.84638 LUMO: 1.90480 factor:1 | 1 (-1.77824) | 1 | 1 |
| G: -5715.18379 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.91815 HOMO: -6.82462 LUMO: 1.70888 factor:1 | 1 (-2.36867) | 1 | 1 |
| G: -5715.18379 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.84490 HOMO: -6.82734 LUMO: 2.12521 factor:1 | 1 (-2.29542) | 1 | 1 |
| G: -5715.18379 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.46813 HOMO: -6.94435 LUMO: 1.87214 factor:1 | 1 (-1.91865) | 1 | 1 |
| G: -5715.18379 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.32777 HOMO: -6.98516 LUMO: 2.51433 factor:1 | 1 (-1.77829) | 1 | 1 |
| G: -5715.18379 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.23424 HOMO: -6.74026 LUMO: 2.15514 factor:1 | 1 (-2.68476) | 1 | 1 |
| G: -5715.18379 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.21448 HOMO: -6.93618 LUMO: 2.54426 factor:1 | 1 (-2.66500) | 1 | 1 |
| G: -5715.18379 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.14776 HOMO: -6.28583 LUMO: 2.53610 factor:1 | 1 (-2.59828) | -1 | -1 |
| G: -5715.18379 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.15124 HOMO: -6.56883 LUMO: 1.94834 factor:1 | 1 (-2.60176) | 1 | 1 |
| G: -5715.18379 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.90947 HOMO: -7.08584 LUMO: 1.99187 factor:1 | 1 (-2.35999) | 1 | 1 |
| G: -5715.18379 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.33721 HOMO: -6.19059 LUMO: 1.99732 factor:1 | 1 (-2.78772) | -1 | -1 |
| G: -5715.18379 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.31620 HOMO: -6.78108 LUMO: 2.03813 factor:1 | 1 (-2.76672) | 1 | 1 |
| G: -5715.18379 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.05798 HOMO: -6.82189 LUMO: 1.77418 factor:1 | 1 (-0.50850) | 1 | 1 |
| G: -5715.18379 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11979.83379 HOMO: -6.45454 LUMO: 1.78779 factor:1 | 1 (-0.28430) | -1 | -1 |
| G: -5715.18379 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.03261 HOMO: -6.84366 LUMO: 1.77690 factor:1 | 1 (-1.48313) | 1 | 1 |
| G: -5715.18379 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.28121 HOMO: -6.74026 LUMO: 1.67622 factor:1 | 1 (-1.73173) | 1 | 1 |
| G: -5715.18379 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.88871 HOMO: -6.76475 LUMO: 2.40277 factor:1 | 1 (-2.33923) | 1 | 1 |
| G: -5715.18379 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.76577 HOMO: -6.65863 LUMO: 1.86670 factor:1 | 1 (-2.21629) | 1 | 1 |
| G: -5715.18379 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.90763 HOMO: -6.50080 LUMO: 1.93201 factor:1 | 1 (-1.35815) | -1 | -1 |
| G: -5715.18379 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.93928 HOMO: -6.34842 LUMO: 1.70888 factor:1 | 1 (-1.38979) | -1 | -1 |
| G: -5715.18379 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.81458 HOMO: -6.60692 LUMO: 2.20140 factor:1 | 1 (-2.26510) | 1 | 1 |
| G: -5715.18379 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.64138 HOMO: -6.74026 LUMO: 2.14970 factor:1 | 1 (-2.09190) | 1 | 1 |
| G: -5715.18379 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.69145 HOMO: -6.63686 LUMO: 2.17419 factor:1 | 1 (-2.14197) | 1 | 1 |
| G: -5715.18379 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.68992 HOMO: -6.81917 LUMO: 2.10072 factor:1 | 1 (-3.14044) | 1 | -1 |
| G: -5715.18379 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.91232 HOMO: -6.92802 LUMO: 2.04358 factor:1 | 1 (-3.36284) | 1 | 1 |
| G: -5715.18379 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.10942 HOMO: -6.56067 LUMO: -0.47620 factor:1 | 1 (-2.55994) | -1 | -1 |
| G: -5715.18379 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.10528 HOMO: -6.56611 LUMO: -0.77008 factor:1 | 1 (-2.55580) | -1 | -1 |
| G: -5715.18379 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.12670 HOMO: -6.78380 LUMO: -0.64763 factor:1 | 1 (-2.57722) | -1 | -1 |
| G: -5715.18379 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.20532 HOMO: -6.51985 LUMO: -0.24490 factor:1 | 1 (-1.65584) | -1 | -1 |
| G: -5715.18379 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.22957 HOMO: -6.52529 LUMO: -0.27483 factor:1 | 1 (-1.68009) | -1 | -1 |
| G: -5715.18379 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.80365 HOMO: -7.10489 LUMO: -0.62586 factor:1 | 1 (-2.25416) | -1 | -1 |
| G: -5715.18379 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.20712 HOMO: -7.18108 LUMO: 0.48980 factor:1 | 1 (-1.65764) | -1 | -1 |
| G: -5715.18379 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.97222 HOMO: -7.14299 LUMO: -0.63947 factor:1 | 1 (-2.42274) | -1 | -1 |
| G: -5715.18379 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.09429 HOMO: -6.70761 LUMO: -0.54423 factor:1 | 1 (-2.54481) | -1 | -1 |
| G: -5715.18379 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.20402 HOMO: -7.32258 LUMO: -1.03675 factor:1 | 1 (-1.65453) | -1 | -1 |
| G: -5715.18379 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.24799 HOMO: -6.65046 LUMO: -0.41361 factor:1 | 1 (-1.69851) | -1 | -1 |
| G: -5715.18379 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.45441 HOMO: -6.76475 LUMO: -0.60137 factor:1 | 1 (-1.90493) | -1 | -1 |
| G: -5715.18379 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.84090 HOMO: -6.77836 LUMO: -0.54423 factor:1 | 1 (-2.29142) | -1 | -1 |
| G: -5715.18379 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.20804 HOMO: -7.52395 LUMO: 0.26395 factor:1 | 1 (-1.65856) | -1 | -1 |
| G: -5715.18379 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.53135 HOMO: -6.93890 LUMO: -0.72382 factor:1 | 1 (-0.98187) | -1 | -1 |
| G: -5715.18379 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.83669 HOMO: -6.72938 LUMO: -0.47348 factor:1 | 1 (-1.28721) | -1 | -1 |
| G: -5715.18379 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.07894 HOMO: -6.66951 LUMO: -0.40817 factor:1 | 1 (-2.52946) | -1 | -1 |
| G: -5715.18379 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.85535 HOMO: -6.60420 LUMO: -0.19320 factor:1 | 1 (-2.30587) | -1 | -1 |
| G: -5715.18379 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.16701 HOMO: -6.67495 LUMO: -0.27211 factor:1 | 1 (-1.61753) | -1 | -1 |
| G: -5715.18379 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.05569 HOMO: -7.23823 LUMO: -0.62858 factor:1 | 1 (-1.50620) | -1 | -1 |
| G: -5715.18379 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.59764 HOMO: -7.27088 LUMO: 0.53334 factor:1 | 1 (-1.04816) | -1 | -1 |
| G: -5715.18379 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11983.26721 HOMO: -7.20013 LUMO: 0.59049 factor:1 | 1 (-3.71773) | -1 | -1 |
| G: -5715.18379 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.51599 HOMO: -6.60148 LUMO: -0.20953 factor:1 | 1 (-2.96650) | -1 | -1 |
| G: -5715.18379 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11983.22079 HOMO: -6.69400 LUMO: -0.51974 factor:1 | 1 (-3.67131) | -1 | -1 |
| G: -5715.18379 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11983.22125 HOMO: -7.40422 LUMO: -0.98777 factor:1 | 1 (-3.67177) | -1 | -1 |
| G: -5715.18379 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.53743 HOMO: -6.88176 LUMO: -0.71022 factor:1 | 1 (-2.98795) | -1 | -1 |
| G: -5715.18379 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.97954 HOMO: -6.86271 LUMO: -0.59321 factor:1 | 1 (-2.43006) | -1 | -1 |
| G: -5715.18379 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.96212 HOMO: -6.73754 LUMO: -0.55239 factor:1 | 1 (-2.41264) | -1 | -1 |
| G: -5715.18379 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.11261 HOMO: -6.71033 LUMO: 1.57010 factor:1 | 1 (-1.56313) | -1 | -1 |
| G: -5715.18379 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.51686 HOMO: -6.69672 LUMO: 1.68711 factor:1 | 1 (-1.96738) | 1 | 1 |
| G: -5715.18379 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.69772 HOMO: -6.67495 LUMO: 2.03813 factor:1 | 1 (-1.14824) | 1 | 1 |
| G: -5715.18379 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.11125 HOMO: -6.54434 LUMO: 1.83677 factor:1 | 1 (-1.56177) | -1 | -1 |
| G: -5715.18379 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.99669 HOMO: -6.57155 LUMO: 1.77146 factor:1 | 1 (-1.44721) | 1 | 1 |
| G: -5715.18379 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11983.21692 HOMO: -6.76747 LUMO: 1.87759 factor:1 | 1 (-3.66744) | 1 | 1 |
| G: -5715.18379 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11983.18732 HOMO: -6.58243 LUMO: 1.61364 factor:1 | 1 (-3.63784) | 1 | 1 |
| G: -5715.18379 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.43484 HOMO: -6.61781 LUMO: 2.13881 factor:1 | 1 (-2.88536) | 1 | 1 |
| G: -5715.18379 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.37035 HOMO: -6.62597 LUMO: 2.00276 factor:1 | 1 (-2.82087) | 1 | 1 |
| G: -5715.18379 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11983.11692 HOMO: -7.01237 LUMO: 1.95922 factor:1 | 1 (-3.56744) | 1 | 1 |
| G: -5715.18379 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.86164 HOMO: -7.03959 LUMO: 2.16875 factor:1 | 1 (-1.31216) | 1 | 1 |
| G: -5715.18379 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.73241 HOMO: -6.83278 LUMO: 1.91296 factor:1 | 1 (-2.18292) | 1 | 1 |
| G: -5715.18379 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.97914 HOMO: -6.40012 LUMO: 1.95650 factor:1 | 1 (-1.42966) | -1 | -1 |
| G: -5715.18379 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11983.18261 HOMO: -6.50080 LUMO: 1.73337 factor:1 | 1 (-3.63313) | -1 | -1 |
| G: -5715.18379 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11983.21145 HOMO: -6.95795 LUMO: 2.28848 factor:1 | 1 (-3.66197) | 1 | 1 |
| G: -5715.18379 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.35974 HOMO: -6.63686 LUMO: 2.20140 factor:1 | 1 (-2.81026) | 1 | -1 |
| G: -5715.18379 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.23476 HOMO: -6.57427 LUMO: 1.87214 factor:1 | 1 (-2.68527) | 1 | -1 |
| G: -5715.18379 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.86739 HOMO: -6.38379 LUMO: 2.32113 factor:1 | 1 (-3.31791) | -1 | -1 |
| G: -5715.18379 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.89505 HOMO: -6.63958 LUMO: 2.04902 factor:1 | 1 (-2.34557) | 1 | 1 |
| G: -5715.18379 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.05340 HOMO: -6.70216 LUMO: 1.93201 factor:1 | 1 (-1.50392) | 1 | 1 |
| G: -5715.18379 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.45545 HOMO: -6.80557 LUMO: 2.23678 factor:1 | 1 (-1.90597) | 1 | 1 |
| G: -5715.18379 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.87606 HOMO: -6.72938 LUMO: 2.28304 factor:1 | 1 (-1.32658) | 1 | 1 |
| G: -5715.18379 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.09052 HOMO: -6.56067 LUMO: 1.66806 factor:1 | 1 (-1.54104) | -1 | -1 |
| G: -5715.18379 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.98212 HOMO: -6.95523 LUMO: 2.33474 factor:1 | 1 (-2.43264) | 1 | 1 |
| G: -5715.18379 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.05272 HOMO: -6.59876 LUMO: 2.30480 factor:1 | 1 (-1.50324) | 1 | 1 |
| G: -5715.18379 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.94364 HOMO: -6.87360 LUMO: 1.75786 factor:1 | 1 (-3.39416) | 1 | 1 |
| G: -5715.18379 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.13369 HOMO: -7.06408 LUMO: 1.99187 factor:1 | 1 (-2.58421) | 1 | 1 |
| G: -5715.18379 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.85839 HOMO: -6.95795 LUMO: 1.88847 factor:1 | 1 (-3.30890) | 1 | 1 |
| G: -5715.18379 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.01576 HOMO: -6.85455 LUMO: 1.63813 factor:1 | 1 (-2.46628) | 1 | 1 |
| G: -5715.18379 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.64974 HOMO: -7.09129 LUMO: 2.31569 factor:1 | 1 (-2.10026) | 1 | 1 |
| G: -5715.18379 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.86315 HOMO: -6.91441 LUMO: 1.68983 factor:1 | 1 (-3.31367) | 1 | 1 |
| G: -5715.18379 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.97467 HOMO: -6.89809 LUMO: 2.23678 factor:1 | 1 (-2.42519) | 1 | 1 |
| G: -5715.18379 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.71474 HOMO: -6.78652 LUMO: 1.98371 factor:1 | 1 (-3.16526) | 1 | -1 |
| G: -5715.18379 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11979.55400 HOMO: -6.94707 LUMO: 2.23678 factor:1 | 1 (-0.00452) | 1 | 1 |
| G: -5715.18379 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.76175 HOMO: -7.07224 LUMO: 2.13337 factor:1 | 1 (-1.21227) | 1 | 1 |
| G: -5715.18379 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.50044 HOMO: -6.94979 LUMO: 2.28031 factor:1 | 1 (-0.95096) | 1 | 1 |
| G: -5715.18379 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.61963 HOMO: -6.60965 LUMO: 2.20412 factor:1 | 1 (-3.07015) | 1 | 1 |
| G: -5715.18379 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.12343 HOMO: -6.87360 LUMO: 2.40277 factor:1 | 1 (-2.57395) | 1 | -1 |
| G: -5715.18379 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.69836 HOMO: -6.92802 LUMO: 1.89663 factor:1 | 1 (-3.14887) | 1 | -1 |
| G: -5715.18379 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.28771 HOMO: -6.88448 LUMO: 2.02725 factor:1 | 1 (-2.73823) | 1 | 1 |
| G: -5715.18379 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.42878 HOMO: -6.69128 LUMO: 1.55105 factor:1 | 1 (-1.87930) | -1 | -1 |
| G: -5715.18379 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.18502 HOMO: -6.54978 LUMO: 1.93201 factor:1 | 1 (-1.63554) | -1 | -1 |
| G: -5715.18379 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.33984 HOMO: -6.19331 LUMO: 1.46941 factor:1 | 1 (-0.79035) | -1 | -1 |
| G: -5715.18379 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.14395 HOMO: -6.55794 LUMO: 1.89663 factor:1 | 1 (-2.59447) | -1 | -1 |
| G: -5715.18379 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.14391 HOMO: -6.07630 LUMO: 1.94289 factor:1 | 1 (-1.59442) | -1 | -1 |
| G: -5715.18379 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.83595 HOMO: -7.46408 LUMO: 0.31565 factor:1 | 1 (-2.28646) | -1 | -1 |
| G: -5715.18379 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.23805 HOMO: -6.63958 LUMO: -0.61770 factor:1 | 1 (-2.68857) | -1 | -1 |
| G: -5715.18379 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.30366 HOMO: -6.81101 LUMO: -0.57960 factor:1 | 1 (-1.75418) | -1 | -1 |
| G: -5715.18379 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.05132 HOMO: -6.74298 LUMO: -0.57960 factor:1 | 1 (-2.50184) | -1 | -1 |
| G: -5715.18379 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.14976 HOMO: -6.63686 LUMO: -0.42994 factor:1 | 1 (-1.60027) | -1 | -1 |
| G: -5715.18379 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.91545 HOMO: -6.60965 LUMO: -0.41089 factor:1 | 1 (-3.36597) | -1 | -1 |
| G: -5715.18379 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11983.31804 HOMO: -6.60692 LUMO: -0.80274 factor:1 | 1 (-3.76856) | -1 | -1 |
| G: -5715.18379 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.10254 HOMO: -6.58788 LUMO: -0.78097 factor:1 | 1 (-2.55305) | -1 | -1 |
| G: -5715.18379 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.30828 HOMO: -6.67767 LUMO: -0.48436 factor:1 | 1 (-2.75880) | -1 | -1 |
| G: -5715.18379 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.65275 HOMO: -6.63141 LUMO: -0.40545 factor:1 | 1 (-3.10327) | -1 | -1 |
| G: -5715.18379 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.34401 HOMO: -6.62053 LUMO: -0.83811 factor:1 | 1 (-2.79453) | -1 | -1 |
| G: -5715.18379 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11983.15521 HOMO: -6.59604 LUMO: -0.35375 factor:1 | 1 (-3.60573) | -1 | -1 |
| G: -5715.18379 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.82962 HOMO: -6.34297 LUMO: -0.39729 factor:1 | 1 (-3.28014) | -1 | -1 |
| G: -5715.18379 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.47463 HOMO: -6.67223 LUMO: 1.97827 factor:1 | 1 (-1.92515) | 1 | 1 |
| G: -5715.18379 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.39918 HOMO: -6.40012 LUMO: 1.89935 factor:1 | 1 (-0.84970) | -1 | -1 |
| G: -5715.18379 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.34585 HOMO: -6.74842 LUMO: 1.97283 factor:1 | 1 (-0.79637) | 1 | -1 |
| G: -5715.18379 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.21040 HOMO: -6.76747 LUMO: 2.17147 factor:1 | 1 (-2.66092) | 1 | 1 |
| G: -5715.18379 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.35917 HOMO: -6.72121 LUMO: 1.55649 factor:1 | 1 (-1.80969) | -1 | -1 |
| G: -5715.18379 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.24926 HOMO: -6.97700 LUMO: 2.04085 factor:1 | 1 (-2.69978) | 1 | 1 |
| G: -5715.18379 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.48342 HOMO: -7.06680 LUMO: 2.04085 factor:1 | 1 (-1.93394) | 1 | -1 |
| G: -5715.18379 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.88465 HOMO: -7.09673 LUMO: 2.35106 factor:1 | 1 (-2.33517) | 1 | 1 |
| G: -5715.18379 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.33440 HOMO: -6.83006 LUMO: 2.14970 factor:1 | 1 (-2.78492) | 1 | 1 |
| G: -5715.18379 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11983.50096 HOMO: -6.72665 LUMO: 2.20140 factor:1 | 1 (-3.95147) | 1 | -1 |
| G: -5715.18379 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.48741 HOMO: -6.77291 LUMO: 2.34562 factor:1 | 1 (-2.93793) | 1 | -1 |
| G: -5715.18379 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11983.41268 HOMO: -6.73754 LUMO: 2.00276 factor:1 | 1 (-3.86320) | 1 | -1 |
| G: -5715.18379 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.80342 HOMO: -7.04231 LUMO: 1.92112 factor:1 | 1 (-3.25394) | 1 | -1 |
| G: -5715.18379 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.19413 HOMO: -6.83822 LUMO: 1.72248 factor:1 | 1 (-2.64465) | 1 | 1 |
| G: -5715.18379 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.91186 HOMO: -6.57971 LUMO: 2.16603 factor:1 | 1 (-3.36237) | 1 | -1 |
| G: -5715.18379 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.48714 HOMO: -6.80013 LUMO: 1.88575 factor:1 | 1 (-2.93766) | 1 | 1 |
| G: -5715.18379 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11983.20430 HOMO: -6.93618 LUMO: 2.18235 factor:1 | 1 (-3.65482) | 1 | 1 |
| G: -5715.18379 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.40970 HOMO: -6.54706 LUMO: 1.91024 factor:1 | 1 (-2.86022) | -1 | -1 |
| G: -5715.18379 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.32942 HOMO: -7.06952 LUMO: 2.18507 factor:1 | 1 (-2.77994) | 1 | 1 |
| G: -5715.18379 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.97590 HOMO: -7.05047 LUMO: 1.82044 factor:1 | 1 (-1.42642) | 1 | 1 |
| G: -5715.18379 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.11610 HOMO: -6.87632 LUMO: 1.92657 factor:1 | 1 (-1.56661) | 1 | 1 |
| G: -5715.18379 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.85676 HOMO: -6.58788 LUMO: 1.91568 factor:1 | 1 (-2.30728) | 1 | -1 |
| G: -5715.18379 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.99497 HOMO: -7.17292 LUMO: 1.90752 factor:1 | 1 (-2.44549) | 1 | 1 |
| G: -5715.18379 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.87799 HOMO: -6.93890 LUMO: 1.80684 factor:1 | 1 (-2.32851) | 1 | 1 |
| G: -5715.18379 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.19143 HOMO: -7.10761 LUMO: 2.20956 factor:1 | 1 (-2.64195) | 1 | 1 |
| G: -5715.18379 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.66078 HOMO: -6.85727 LUMO: 2.13609 factor:1 | 1 (-3.11130) | 1 | -1 |
| G: -5715.18379 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.94437 HOMO: -6.64502 LUMO: 1.38506 factor:1 | 1 (-3.39489) | -1 | -1 |
| G: -5715.18379 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.10313 HOMO: -6.87360 LUMO: 1.15648 factor:1 | 1 (-2.55365) | -1 | -1 |
| G: -5715.18379 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11983.18266 HOMO: -6.67223 LUMO: 2.07351 factor:1 | 1 (-3.63318) | 1 | 1 |
| G: -5715.18379 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.34613 HOMO: -6.29671 LUMO: 2.43270 factor:1 | 1 (-2.79665) | -1 | -1 |
| G: -5715.18379 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.23067 HOMO: -6.90897 LUMO: 2.28848 factor:1 | 1 (-2.68119) | 1 | 1 |
| G: -5715.18379 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.87020 HOMO: -7.04231 LUMO: 1.70071 factor:1 | 1 (-2.32072) | 1 | 1 |
| G: -5715.18379 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.23053 HOMO: -6.69944 LUMO: 1.94834 factor:1 | 1 (-0.68105) | 1 | 1 |
| G: -5715.18379 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.91873 HOMO: -6.56067 LUMO: 2.20956 factor:1 | 1 (-1.36925) | -1 | -1 |
| G: -5715.18379 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.98747 HOMO: -6.65046 LUMO: 2.06807 factor:1 | 1 (-1.43799) | 1 | -1 |
| G: -5715.18379 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.02002 HOMO: -7.08584 LUMO: 1.98915 factor:1 | 1 (-0.47054) | 1 | 1 |
| G: -5715.18379 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.23739 HOMO: -6.69400 LUMO: 2.09256 factor:1 | 1 (-2.68791) | 1 | 1 |
| G: -5715.18379 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.56652 HOMO: -6.62869 LUMO: 2.16331 factor:1 | 1 (-3.01704) | 1 | 1 |
| G: -5715.18379 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.75551 HOMO: -6.85183 LUMO: 2.16058 factor:1 | 1 (-2.20603) | 1 | 1 |
| G: -5715.18379 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.15837 HOMO: -6.54706 LUMO: 1.92384 factor:1 | 1 (-2.60889) | -1 | -1 |
| G: -5715.18379 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.84795 HOMO: -6.84366 LUMO: 2.48984 factor:1 | 1 (-2.29846) | 1 | 1 |
| G: -5715.18379 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.90439 HOMO: -6.77291 LUMO: 2.46263 factor:1 | 1 (-1.35491) | 1 | 1 |
| G: -5715.18379 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.22848 HOMO: -7.01782 LUMO: 2.31025 factor:1 | 1 (-1.67900) | 1 | 1 |
| G: -5715.18379 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.01925 HOMO: -6.94707 LUMO: 2.29664 factor:1 | 1 (-1.46977) | 1 | 1 |
| G: -5715.18379 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.13911 HOMO: -6.64230 LUMO: 1.97283 factor:1 | 1 (-2.58963) | 1 | 1 |
| G: -5715.18379 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.33213 HOMO: -6.47359 LUMO: 2.20412 factor:1 | 1 (-1.78265) | -1 | -1 |
| G: -5715.18379 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.93345 HOMO: -6.90625 LUMO: 1.92384 factor:1 | 1 (-1.38397) | 1 | 1 |
| G: -5715.18379 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.03988 HOMO: -7.17020 LUMO: 2.06807 factor:1 | 1 (-1.49039) | 1 | 1 |
| G: -5715.18379 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.89857 HOMO: -6.65046 LUMO: 2.20956 factor:1 | 1 (-1.34909) | 1 | -1 |
| G: -5715.18379 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.04945 HOMO: -7.07496 LUMO: 1.82861 factor:1 | 1 (-2.49996) | 1 | 1 |
| G: -5715.18379 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.16772 HOMO: -6.83006 LUMO: 2.14970 factor:1 | 1 (-1.61823) | 1 | -1 |
| G: -5715.18379 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.91530 HOMO: -6.92802 LUMO: 1.99187 factor:1 | 1 (-1.36582) | 1 | 1 |
| G: -5715.18379 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.07951 HOMO: -6.69672 LUMO: 2.36739 factor:1 | 1 (-2.53003) | 1 | -1 |
| G: -5715.18379 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.11169 HOMO: -7.13755 LUMO: 2.00276 factor:1 | 1 (-1.56221) | 1 | 1 |
| G: -5715.18379 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.76381 HOMO: -6.92530 LUMO: 2.25582 factor:1 | 1 (-2.21433) | 1 | 1 |
| G: -5715.18379 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.67865 HOMO: -6.77564 LUMO: 1.97827 factor:1 | 1 (-1.12916) | 1 | 1 |
| G: -5715.18379 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.56988 HOMO: -6.87904 LUMO: 1.60003 factor:1 | 1 (-1.02040) | 1 | 1 |
| G: -5715.18379 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.82227 HOMO: -6.62869 LUMO: 1.90480 factor:1 | 1 (-1.27279) | 1 | 1 |
| G: -5715.18379 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.76356 HOMO: -6.71033 LUMO: 1.54833 factor:1 | 1 (-2.21408) | -1 | -1 |
| G: -5715.18379 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.67567 HOMO: -6.74298 LUMO: 1.47486 factor:1 | 1 (-2.12619) | -1 | -1 |
| G: -5715.18379 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.49193 HOMO: -6.77019 LUMO: 1.90480 factor:1 | 1 (-2.94245) | 1 | 1 |
| G: -5715.18379 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.87818 HOMO: -6.70489 LUMO: 1.99459 factor:1 | 1 (-2.32870) | 1 | 1 |
| G: -5715.18379 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.58193 HOMO: -6.73482 LUMO: 2.08711 factor:1 | 1 (-2.03245) | 1 | 1 |
| G: -5715.18379 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.51027 HOMO: -6.46543 LUMO: 1.73881 factor:1 | 1 (-2.96079) | -1 | -1 |
| G: -5715.18379 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11983.15937 HOMO: -6.96067 LUMO: 2.26127 factor:1 | 1 (-3.60989) | 1 | 1 |
| G: -5715.18379 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.46986 HOMO: -6.67767 LUMO: 2.10616 factor:1 | 1 (-2.92038) | 1 | 1 |
| G: -5715.18379 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.99442 HOMO: -6.28855 LUMO: 2.35923 factor:1 | 1 (-3.44493) | -1 | -1 |
| G: -5715.18379 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.30687 HOMO: -6.80285 LUMO: 1.62724 factor:1 | 1 (-2.75738) | 1 | 1 |
| G: -5715.18379 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.41778 HOMO: -6.85455 LUMO: 2.23133 factor:1 | 1 (-2.86830) | 1 | 1 |
| G: -5715.18379 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11983.17616 HOMO: -6.51713 LUMO: 2.33474 factor:1 | 1 (-3.62668) | -1 | -1 |
| G: -5715.18379 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11983.42188 HOMO: -6.88176 LUMO: 2.15242 factor:1 | 1 (-3.87240) | 1 | 1 |
| G: -5715.18379 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.53786 HOMO: -6.54434 LUMO: 2.32113 factor:1 | 1 (-2.98838) | -1 | -1 |
| G: -5715.18379 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.60565 HOMO: -6.62597 LUMO: 2.24222 factor:1 | 1 (-3.05617) | 1 | 1 |
| G: -5715.18379 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.50001 HOMO: -6.74570 LUMO: 2.19868 factor:1 | 1 (-2.95053) | 1 | 1 |
| G: -5715.18379 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.41197 HOMO: -6.62869 LUMO: 1.98915 factor:1 | 1 (-0.86249) | 1 | 1 |
| G: -5715.18379 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.54894 HOMO: -6.64502 LUMO: 2.13881 factor:1 | 1 (-2.99946) | 1 | 1 |
| G: -5715.18379 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.16841 HOMO: -6.95795 LUMO: 1.82316 factor:1 | 1 (-2.61893) | 1 | 1 |
| G: -5715.18379 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.26625 HOMO: -6.77291 LUMO: 1.36329 factor:1 | 1 (-1.71677) | -1 | -1 |
| G: -5715.18379 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.61645 HOMO: -6.45726 LUMO: 1.73064 factor:1 | 1 (-3.06697) | -1 | -1 |
| G: -5715.18379 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.59185 HOMO: -6.49264 LUMO: 1.77418 factor:1 | 1 (-3.04237) | -1 | -1 |
| G: -5715.18379 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.38218 HOMO: -6.60420 LUMO: 2.20956 factor:1 | 1 (-0.83270) | 1 | 1 |
| G: -5715.18379 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.44733 HOMO: -6.56067 LUMO: 2.05718 factor:1 | 1 (-2.89785) | -1 | -1 |
| G: -5715.18379 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.06987 HOMO: -6.62597 LUMO: 1.70343 factor:1 | 1 (-0.52039) | 1 | 1 |
| G: -5715.18379 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11979.88524 HOMO: -6.69400 LUMO: 2.16875 factor:1 | 1 (-0.33576) | 1 | 1 |
| G: -5715.18379 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.31586 HOMO: -6.63958 LUMO: 2.11977 factor:1 | 1 (-0.76638) | 1 | 1 |
| G: -5715.18379 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.92588 HOMO: -6.92802 LUMO: 1.82044 factor:1 | 1 (-2.37640) | 1 | -1 |
| G: -5715.18379 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.18714 HOMO: -6.56339 LUMO: 2.30480 factor:1 | 1 (-1.63766) | -1 | -1 |
| G: -5715.18379 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11979.97948 HOMO: -6.63958 LUMO: 1.91024 factor:1 | 1 (-0.42999) | 1 | -1 |
| G: -5715.18379 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.39869 HOMO: -6.93074 LUMO: 2.05446 factor:1 | 1 (-0.84921) | 1 | 1 |
| G: -5715.18379 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.71898 HOMO: -6.61509 LUMO: 2.03813 factor:1 | 1 (-3.16950) | 1 | 1 |
| G: -5715.18379 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.23348 HOMO: -6.61237 LUMO: 1.91296 factor:1 | 1 (-2.68400) | 1 | -1 |
| G: -5715.18379 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.30989 HOMO: -6.86815 LUMO: 1.95378 factor:1 | 1 (-2.76040) | 1 | 1 |
| G: -5715.18379 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.25359 HOMO: -6.63686 LUMO: 1.70888 factor:1 | 1 (-2.70410) | 1 | 1 |
| G: -5715.18379 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.04606 HOMO: -6.57971 LUMO: 2.20140 factor:1 | 1 (-0.49658) | 1 | -1 |
| G: -5715.18379 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11979.83213 HOMO: -6.41100 LUMO: 1.96738 factor:1 | 1 (-0.28264) | -1 | -1 |
| G: -5715.18379 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.29966 HOMO: -6.90081 LUMO: 1.65989 factor:1 | 1 (-1.75018) | 1 | 1 |
| G: -5715.18379 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.95464 HOMO: -6.68312 LUMO: 1.97827 factor:1 | 1 (-2.40516) | 1 | -1 |
| G: -5715.18379 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.04796 HOMO: -6.65318 LUMO: 2.10888 factor:1 | 1 (-1.49848) | 1 | -1 |
| G: -5715.18379 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.73859 HOMO: -6.62053 LUMO: 2.28848 factor:1 | 1 (-1.18911) | 1 | -1 |
| G: -5715.18379 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.48553 HOMO: -6.65863 LUMO: 2.29664 factor:1 | 1 (-0.93604) | 1 | -1 |
| G: -5715.18379 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.37834 HOMO: -6.63958 LUMO: 2.07623 factor:1 | 1 (-0.82886) | 1 | -1 |
| G: -5715.18379 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.16827 HOMO: -6.58243 LUMO: 2.20684 factor:1 | 1 (-0.61879) | 1 | 1 |
| G: -5715.18379 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.08424 HOMO: -6.59332 LUMO: 2.05174 factor:1 | 1 (-0.53476) | 1 | -1 |
| G: -5715.18379 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.35264 HOMO: -6.95251 LUMO: 2.20140 factor:1 | 1 (-1.80316) | 1 | 1 |
| G: -5715.18379 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.18825 HOMO: -6.84638 LUMO: 2.39732 factor:1 | 1 (-2.63877) | 1 | 1 |
| G: -5715.18379 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.02574 HOMO: -6.86815 LUMO: 2.47896 factor:1 | 1 (-2.47626) | 1 | 1 |
| G: -5715.18379 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.14342 HOMO: -7.00693 LUMO: 2.43270 factor:1 | 1 (-1.59393) | 1 | 1 |
| G: -5715.18379 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.08096 HOMO: -6.58788 LUMO: 2.30208 factor:1 | 1 (-2.53148) | 1 | 1 |
| G: -5715.18379 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.20192 HOMO: -6.63958 LUMO: 2.28031 factor:1 | 1 (-1.65244) | 1 | 1 |
| G: -5715.18379 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.11888 HOMO: -6.74570 LUMO: 2.28304 factor:1 | 1 (-0.56940) | 1 | 1 |
| G: -5715.18379 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.16253 HOMO: -6.78380 LUMO: 2.16331 factor:1 | 1 (-0.61305) | 1 | 1 |
| G: -5715.18379 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.73946 HOMO: -6.52529 LUMO: 2.05718 factor:1 | 1 (-1.18998) | -1 | -1 |
| G: -5715.18379 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.63413 HOMO: -6.41644 LUMO: 1.65445 factor:1 | 1 (-1.08465) | -1 | -1 |
| G: -5715.18379 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11979.95567 HOMO: -6.34570 LUMO: 1.22451 factor:1 | 1 (-0.40618) | -1 | -1 |
| G: -5715.18379 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.19428 HOMO: -6.14433 LUMO: 1.85582 factor:1 | 1 (-0.64480) | -1 | -1 |
| G: -5715.18379 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11979.49718 HOMO: -6.62053 LUMO: 1.92112 factor:1 | -1 (0.05230) | 1 | -1 |
| G: -5715.18379 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11979.18738 HOMO: -6.63414 LUMO: 1.61908 factor:1 | -1 (0.36210) | 1 | 1 |
| G: -5715.18379 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.06731 HOMO: -6.75931 LUMO: 1.87214 factor:1 | 1 (-0.51783) | 1 | 1 |
| G: -5715.18379 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.65767 HOMO: -6.55794 LUMO: 1.77418 factor:1 | 1 (-1.10818) | -1 | -1 |
| G: -5715.18379 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.62218 HOMO: -6.52801 LUMO: 1.82044 factor:1 | 1 (-1.07270) | -1 | -1 |
| G: -5715.18379 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.87040 HOMO: -6.77564 LUMO: 1.97827 factor:1 | 1 (-1.32092) | 1 | 1 |
| G: -5715.18379 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.74635 HOMO: -6.93890 LUMO: 1.81228 factor:1 | 1 (-1.19687) | 1 | 1 |
| G: -5715.18379 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.40139 HOMO: -6.85455 LUMO: 1.75513 factor:1 | 1 (-0.85191) | 1 | 1 |
| G: -5715.18379 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.61100 HOMO: -6.86815 LUMO: 1.64629 factor:1 | 1 (-1.06152) | 1 | 1 |
| G: -5715.18379 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11979.99422 HOMO: -6.98516 LUMO: 1.84765 factor:1 | 1 (-0.44474) | 1 | 1 |
| G: -5715.18379 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.96243 HOMO: -6.04637 LUMO: 1.94017 factor:1 | 1 (-1.41295) | -1 | -1 |
| G: -5715.18379 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.85658 HOMO: -6.86271 LUMO: 2.11977 factor:1 | 1 (-1.30710) | 1 | -1 |
| G: -5715.18379 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.67560 HOMO: -6.72938 LUMO: 2.11160 factor:1 | 1 (-1.12612) | 1 | -1 |
| G: -5715.18379 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.61647 HOMO: -7.01782 LUMO: 2.13609 factor:1 | 1 (-1.06699) | 1 | 1 |
| G: -5715.18379 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.00529 HOMO: -6.18515 LUMO: 2.04630 factor:1 | 1 (-1.45581) | -1 | -1 |
| G: -5715.18379 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.14478 HOMO: -6.60965 LUMO: 2.17147 factor:1 | 1 (-1.59529) | 1 | -1 |
| G: -5715.18379 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.34486 HOMO: -6.87360 LUMO: 2.35378 factor:1 | 1 (-1.79538) | 1 | 1 |
| G: -5715.18379 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.12491 HOMO: -6.72938 LUMO: 2.20140 factor:1 | 1 (-1.57543) | 1 | -1 |
| G: -5715.18379 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.92959 HOMO: -6.88448 LUMO: 2.54154 factor:1 | 1 (-1.38011) | 1 | -1 |
| G: -5715.18379 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.52689 HOMO: -6.87087 LUMO: 2.16058 factor:1 | 1 (-0.97741) | 1 | 1 |
| G: -5715.18379 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.45353 HOMO: -7.11306 LUMO: 2.04085 factor:1 | 1 (-0.90404) | 1 | 1 |
| G: -5715.18379 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.41206 HOMO: -6.66951 LUMO: 1.68438 factor:1 | 1 (-0.86257) | 1 | 1 |
| G: -5715.18379 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.32226 HOMO: -7.08312 LUMO: 2.19324 factor:1 | 1 (-0.77278) | 1 | 1 |
| G: -5715.18379 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.10074 HOMO: -6.69128 LUMO: 2.13881 factor:1 | 1 (-2.55126) | 1 | -1 |
| G: -5715.18379 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.64742 HOMO: -6.80285 LUMO: 2.16603 factor:1 | 1 (-3.09793) | 1 | 1 |
| G: -5715.18379 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11983.34318 HOMO: -6.82189 LUMO: 2.46807 factor:1 | 1 (-3.79370) | 1 | 1 |
| G: -5715.18379 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.76614 HOMO: -6.78652 LUMO: 2.12521 factor:1 | 1 (-3.21666) | 1 | 1 |
| G: -5715.18379 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.11750 HOMO: -6.47903 LUMO: 1.70071 factor:1 | 1 (-2.56802) | -1 | -1 |
| G: -5715.18379 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.01951 HOMO: -6.37019 LUMO: 1.24356 factor:1 | 1 (-2.47003) | -1 | -1 |
| G: -5715.18379 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11983.08723 HOMO: -6.69400 LUMO: 1.67350 factor:1 | 1 (-3.53775) | 1 | 1 |
| G: -5715.18379 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11983.07733 HOMO: -7.51851 LUMO: 0.27756 factor:1 | 1 (-3.52785) | -1 | -1 |
| G: -5715.18379 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11983.09491 HOMO: -6.95795 LUMO: -0.72110 factor:1 | 1 (-3.54543) | -1 | -1 |
| G: -5715.18379 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.38651 HOMO: -6.88720 LUMO: -0.67484 factor:1 | 1 (-2.83703) | -1 | -1 |
| G: -5715.18379 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.45819 HOMO: -6.83550 LUMO: -0.57144 factor:1 | 1 (-2.90871) | -1 | -1 |
| G: -5715.18379 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11983.05534 HOMO: -6.80285 LUMO: -0.57144 factor:1 | 1 (-3.50586) | -1 | -1 |
| G: -5715.18379 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11983.47415 HOMO: -6.76475 LUMO: -0.53062 factor:1 | 1 (-3.92467) | -1 | -1 |
| G: -5715.18379 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11983.19978 HOMO: -6.66951 LUMO: 1.74969 factor:1 | 1 (-3.65030) | 1 | 1 |
| G: -5715.18379 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.57245 HOMO: -6.53345 LUMO: 1.89935 factor:1 | 1 (-3.02297) | -1 | -1 |
| G: -5715.18379 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11983.21910 HOMO: -6.65046 LUMO: 2.01364 factor:1 | 1 (-3.66962) | 1 | -1 |
| G: -5715.18379 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11983.65837 HOMO: -6.64230 LUMO: 2.11977 factor:1 | 1 (-4.10889) | 1 | -1 |
| G: -5715.18379 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.55163 HOMO: -6.44910 LUMO: 2.13337 factor:1 | 1 (-3.00215) | -1 | -1 |
| G: -5715.18379 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.85039 HOMO: -7.05591 LUMO: 1.98915 factor:1 | 1 (-3.30090) | 1 | -1 |
| G: -5715.18379 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11983.62621 HOMO: -7.02326 LUMO: 2.49256 factor:1 | 1 (-4.07673) | 1 | 1 |
| G: -5715.18379 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.52436 HOMO: -6.32937 LUMO: 2.51161 factor:1 | 1 (-0.97488) | -1 | -1 |
| G: -5715.18379 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.25452 HOMO: -6.96067 LUMO: 2.20140 factor:1 | 1 (-1.70504) | 1 | 1 |
| G: -5715.18379 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.28350 HOMO: -6.97972 LUMO: 2.55243 factor:1 | 1 (-1.73402) | 1 | 1 |
| G: -5715.18379 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11983.21687 HOMO: -6.72665 LUMO: 2.46535 factor:1 | 1 (-3.66739) | 1 | 1 |
| G: -5715.18379 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.65114 HOMO: -6.41917 LUMO: 2.35106 factor:1 | 1 (-3.10166) | -1 | -1 |
| G: -5715.18379 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11983.24718 HOMO: -6.75114 LUMO: 2.32929 factor:1 | 1 (-3.69770) | 1 | 1 |
| G: -5715.18379 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.82168 HOMO: -6.91713 LUMO: 2.27215 factor:1 | 1 (-3.27220) | 1 | 1 |
| G: -5715.18379 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11983.59957 HOMO: -6.54978 LUMO: 2.00276 factor:1 | 1 (-4.05009) | -1 | -1 |
| G: -5715.18379 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11983.15075 HOMO: -6.62325 LUMO: 2.05990 factor:1 | 1 (-3.60126) | 1 | 1 |
| G: -5715.18379 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.32414 HOMO: -6.86271 LUMO: 2.14970 factor:1 | 1 (-0.77465) | 1 | 1 |
| G: -5715.18379 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.41313 HOMO: -6.77564 LUMO: 2.25855 factor:1 | 1 (-2.86364) | 1 | -1 |
| G: -5715.18379 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.56369 HOMO: -6.71305 LUMO: 1.94561 factor:1 | 1 (-3.01421) | 1 | -1 |
| G: -5715.18379 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.71817 HOMO: -6.75659 LUMO: 1.94561 factor:1 | 1 (-3.16868) | 1 | -1 |
| G: -5715.18379 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.56861 HOMO: -6.94979 LUMO: 2.33474 factor:1 | 1 (-3.01913) | 1 | -1 |
| G: -5715.18379 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.66709 HOMO: -6.85727 LUMO: 2.50345 factor:1 | 1 (-3.11761) | 1 | -1 |
| G: -5715.18379 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.96698 HOMO: -6.87360 LUMO: 2.43270 factor:1 | 1 (-1.41750) | 1 | -1 |
| G: -5715.18379 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.47510 HOMO: -6.57427 LUMO: 2.46807 factor:1 | 1 (-1.92561) | 1 | -1 |
| G: -5715.18379 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.11151 HOMO: -7.16204 LUMO: 2.15242 factor:1 | 1 (-0.56202) | 1 | 1 |
| G: -5715.18379 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.43480 HOMO: -6.62869 LUMO: 2.11432 factor:1 | 1 (-0.88532) | 1 | -1 |
| G: -5715.18379 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.29515 HOMO: -7.05591 LUMO: 2.26671 factor:1 | 1 (-1.74566) | 1 | -1 |
| G: -5715.18379 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.38244 HOMO: -7.13483 LUMO: 1.47758 factor:1 | 1 (-1.83296) | -1 | -1 |
| G: -5715.18379 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.09753 HOMO: -6.72938 LUMO: 1.57282 factor:1 | 1 (-2.54805) | -1 | -1 |
| G: -5715.18379 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.31681 HOMO: -6.17426 LUMO: 1.81228 factor:1 | 1 (-1.76733) | -1 | -1 |
| G: -5715.18379 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.67216 HOMO: -6.65318 LUMO: 1.93473 factor:1 | 1 (-2.12268) | 1 | -1 |
| G: -5715.18379 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.19991 HOMO: -6.18515 LUMO: 2.01364 factor:1 | 1 (-1.65042) | -1 | -1 |
| G: -5715.18379 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11983.05121 HOMO: -7.05591 LUMO: 2.13337 factor:1 | 1 (-3.50172) | 1 | 1 |
| G: -5715.18379 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11983.14049 HOMO: -6.90897 LUMO: 2.29664 factor:1 | 1 (-3.59100) | 1 | -1 |
| G: -5715.18379 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11983.09551 HOMO: -7.11034 LUMO: 2.17147 factor:1 | 1 (-3.54602) | 1 | 1 |
| G: -5715.18379 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.05489 HOMO: -6.82734 LUMO: 2.26671 factor:1 | 1 (-2.50541) | 1 | 1 |
| G: -5715.18379 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.27715 HOMO: -6.34842 LUMO: 2.34562 factor:1 | 1 (-2.72767) | -1 | -1 |
| G: -5715.18379 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.78053 HOMO: -6.62053 LUMO: 2.22861 factor:1 | 1 (-3.23105) | 1 | -1 |
| G: -5715.18379 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.78862 HOMO: -6.80557 LUMO: 2.07079 factor:1 | 1 (-2.23914) | 1 | -1 |
| G: -5715.18379 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.15248 HOMO: -6.60692 LUMO: 2.46263 factor:1 | 1 (-1.60300) | 1 | -1 |
| G: -5715.18379 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.11608 HOMO: -7.02054 LUMO: 2.08711 factor:1 | 1 (-0.56660) | 1 | -1 |
| G: -5715.18379 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.49955 HOMO: -6.78652 LUMO: 2.02453 factor:1 | 1 (-2.95007) | 1 | 1 |
| G: -5715.18379 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.58156 HOMO: -6.51168 LUMO: 2.06534 factor:1 | 1 (-3.03208) | -1 | -1 |
| G: -5715.18379 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.27476 HOMO: -6.50080 LUMO: 2.01636 factor:1 | 1 (-2.72527) | -1 | -1 |
| G: -5715.18379 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.37228 HOMO: -6.54434 LUMO: 1.84493 factor:1 | 1 (-2.82280) | -1 | -1 |
| G: -5715.18379 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.45160 HOMO: -6.47087 LUMO: 1.76330 factor:1 | 1 (-2.90212) | -1 | -1 |
| G: -5715.18379 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.43439 HOMO: -6.78924 LUMO: 2.39460 factor:1 | 1 (-1.88491) | 1 | 1 |
| G: -5715.18379 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.11205 HOMO: -6.59876 LUMO: 1.84493 factor:1 | 1 (-0.56257) | 1 | 1 |
| G: -5715.18379 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.24043 HOMO: -6.41644 LUMO: 2.05174 factor:1 | 1 (-0.69095) | -1 | -1 |
| G: -5715.18379 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.24035 HOMO: -6.52257 LUMO: 2.11160 factor:1 | 1 (-0.69087) | -1 | -1 |
| G: -5715.18379 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.16792 HOMO: -6.90897 LUMO: 2.34018 factor:1 | 1 (-2.61844) | 1 | 1 |
| G: -5715.18379 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.36726 HOMO: -6.97428 LUMO: 1.86126 factor:1 | 1 (-1.81778) | 1 | 1 |
| G: -5715.18379 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.21960 HOMO: -7.13483 LUMO: 2.14698 factor:1 | 1 (-2.67012) | 1 | -1 |
| G: -5715.18379 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.42573 HOMO: -7.16748 LUMO: 2.31841 factor:1 | 1 (-1.87625) | 1 | 1 |
| G: -5715.18379 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.10475 HOMO: -6.87087 LUMO: 2.38916 factor:1 | 1 (-1.55527) | 1 | -1 |
| G: -5715.18379 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.36859 HOMO: -6.93074 LUMO: 2.42181 factor:1 | 1 (-1.81911) | 1 | -1 |
| G: -5715.18379 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.19430 HOMO: -6.90081 LUMO: 2.00276 factor:1 | 1 (-1.64482) | 1 | -1 |
| G: -5715.18379 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.65698 HOMO: -6.99333 LUMO: 2.03541 factor:1 | 1 (-1.10750) | 1 | 1 |
| G: -5715.18379 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.59329 HOMO: -6.89264 LUMO: 1.57554 factor:1 | 1 (-3.04381) | -1 | -1 |
| G: -5715.18379 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.60576 HOMO: -6.48175 LUMO: 1.85854 factor:1 | 1 (-3.05627) | -1 | -1 |
| G: -5715.18379 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11983.55979 HOMO: -6.69400 LUMO: 1.62452 factor:1 | 1 (-4.01031) | 1 | 1 |
| G: -5715.18379 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.41783 HOMO: -6.50896 LUMO: 1.88303 factor:1 | 1 (-2.86835) | -1 | -1 |
| G: -5715.18379 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11983.16645 HOMO: -6.60420 LUMO: 2.05990 factor:1 | 1 (-3.61696) | 1 | 1 |
| G: -5715.18379 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.64192 HOMO: -7.14299 LUMO: 2.07351 factor:1 | 1 (-3.09244) | 1 | 1 |
| G: -5715.18379 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.05013 HOMO: -7.06408 LUMO: 1.81228 factor:1 | 1 (-2.50064) | 1 | 1 |
| G: -5715.18379 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11979.98783 HOMO: -6.67495 LUMO: 1.79595 factor:1 | 1 (-0.43835) | 1 | 1 |
| G: -5715.18379 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.98276 HOMO: -6.45182 LUMO: 2.15786 factor:1 | 1 (-1.43328) | -1 | -1 |
| G: -5715.18379 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.48344 HOMO: -6.93346 LUMO: 2.45719 factor:1 | 1 (-2.93396) | 1 | 1 |
| G: -5715.18379 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.57150 HOMO: -6.50080 LUMO: 2.08167 factor:1 | 1 (-3.02201) | -1 | -1 |
| G: -5715.18379 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.30175 HOMO: -6.83550 LUMO: -0.67484 factor:1 | 1 (-2.75227) | -1 | -1 |
| G: -5715.18379 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.45337 HOMO: -7.04231 LUMO: 0.54151 factor:1 | 1 (-2.90389) | -1 | -1 |
| G: -5715.18379 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.49101 HOMO: -6.79740 LUMO: 1.91296 factor:1 | 1 (-2.94152) | -1 | -1 |
| G: -5715.18379 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.27369 HOMO: -7.35796 LUMO: -1.04220 factor:1 | 1 (-2.72421) | -1 | -1 |
| G: -5715.18379 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.46358 HOMO: -6.62597 LUMO: -0.44082 factor:1 | 1 (-2.91409) | -1 | -1 |
| G: -5715.18379 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.72993 HOMO: -6.45182 LUMO: -0.20409 factor:1 | 1 (-2.18045) | -1 | -1 |
| G: -5715.18379 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.56937 HOMO: -6.51168 LUMO: -0.23130 factor:1 | 1 (-3.01989) | -1 | -1 |
| G: -5715.18379 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.41957 HOMO: -7.14027 LUMO: 0.49797 factor:1 | 1 (-0.87008) | -1 | -1 |
| G: -5715.18379 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.19559 HOMO: -7.55660 LUMO: 0.24762 factor:1 | 1 (-0.64611) | -1 | -1 |
| G: -5715.18379 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.36144 HOMO: -6.88992 LUMO: -0.64763 factor:1 | 1 (-0.81196) | -1 | -1 |
| G: -5715.18379 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.14567 HOMO: -6.72665 LUMO: -0.45987 factor:1 | 1 (-2.59618) | -1 | -1 |
| G: -5715.18379 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.47183 HOMO: -6.72121 LUMO: -0.58232 factor:1 | 1 (-1.92235) | -1 | -1 |
| G: -5715.18379 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.32119 HOMO: -7.26816 LUMO: 0.32926 factor:1 | 1 (-1.77171) | -1 | -1 |
| G: -5715.18379 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.43609 HOMO: -6.57155 LUMO: -0.53606 factor:1 | 1 (-2.88661) | -1 | -1 |
| G: -5715.18379 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.89977 HOMO: -6.50896 LUMO: -0.43810 factor:1 | 1 (-3.35029) | -1 | -1 |
| G: -5715.18379 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.52913 HOMO: -6.73210 LUMO: -0.51430 factor:1 | 1 (-2.97965) | -1 | -1 |
| G: -5715.18379 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.44891 HOMO: -6.77019 LUMO: -0.62858 factor:1 | 1 (-2.89943) | -1 | -1 |
| G: -5715.18379 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.17527 HOMO: -6.82462 LUMO: -0.67484 factor:1 | 1 (-2.62579) | -1 | -1 |
| G: -5715.18379 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.07513 HOMO: -6.79740 LUMO: -0.55511 factor:1 | 1 (-2.52565) | -1 | -1 |
| G: -5715.18379 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.70883 HOMO: -6.79740 LUMO: -0.67756 factor:1 | 1 (-3.15935) | -1 | -1 |
| G: -5715.18379 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.46227 HOMO: -6.75114 LUMO: -0.55239 factor:1 | 1 (-2.91279) | -1 | -1 |
| G: -5715.18379 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.31193 HOMO: -6.49536 LUMO: -0.25307 factor:1 | 1 (-2.76245) | -1 | -1 |
| G: -5715.18379 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.72627 HOMO: -6.48992 LUMO: -0.25034 factor:1 | 1 (-3.17679) | -1 | -1 |
| G: -5715.18379 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.00021 HOMO: -6.52801 LUMO: -0.28028 factor:1 | 1 (-0.45073) | -1 | -1 |
| G: -5715.18379 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.76315 HOMO: -7.22462 LUMO: 0.52518 factor:1 | 1 (-2.21367) | -1 | -1 |
| G: -5715.18379 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.12237 HOMO: -6.59332 LUMO: -0.27211 factor:1 | 1 (-2.57289) | -1 | -1 |
| G: -5715.18379 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.29158 HOMO: -6.57427 LUMO: -0.16871 factor:1 | 1 (-1.74210) | -1 | -1 |
| G: -5715.18379 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.05408 HOMO: -6.71033 LUMO: 1.59187 factor:1 | 1 (-1.50460) | -1 | -1 |
| G: -5715.18379 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.20297 HOMO: -6.72121 LUMO: 2.00004 factor:1 | 1 (-2.65349) | -1 | -1 |
| G: -5715.18379 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.33972 HOMO: -6.61509 LUMO: 1.55921 factor:1 | 1 (-1.79024) | -1 | -1 |
| G: -5715.18379 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.21609 HOMO: -6.55250 LUMO: 1.73064 factor:1 | 1 (-2.66661) | -1 | -1 |
| G: -5715.18379 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.26864 HOMO: -6.66135 LUMO: 2.02181 factor:1 | 1 (-1.71916) | -1 | -1 |
| G: -5715.18379 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.79576 HOMO: -6.84911 LUMO: 1.98099 factor:1 | 1 (-1.24628) | -1 | -1 |
| G: -5715.18379 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.08738 HOMO: -6.66679 LUMO: 1.98371 factor:1 | 1 (-2.53790) | -1 | -1 |
| G: -5715.18379 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.21234 HOMO: -6.67495 LUMO: 2.04085 factor:1 | 1 (-1.66286) | -1 | -1 |
| G: -5715.18379 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.01362 HOMO: -6.89809 LUMO: 1.95106 factor:1 | 1 (-1.46414) | -1 | -1 |
| G: -5715.18379 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.35159 HOMO: -6.50352 LUMO: 1.88847 factor:1 | 1 (-0.80211) | -1 | -1 |
| G: -5715.18379 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.41304 HOMO: -6.93618 LUMO: 2.00004 factor:1 | 1 (-2.86356) | -1 | -1 |
| G: -5715.18379 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.36385 HOMO: -6.50896 LUMO: 1.73609 factor:1 | 1 (-2.81436) | -1 | -1 |
| G: -5715.18379 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.17231 HOMO: -6.69672 LUMO: 2.37283 factor:1 | 1 (-2.62282) | -1 | -1 |
| G: -5715.18379 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.82854 HOMO: -6.65591 LUMO: 2.20684 factor:1 | 1 (-3.27905) | -1 | -1 |
| G: -5715.18379 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.48211 HOMO: -6.23957 LUMO: 1.78507 factor:1 | 1 (-2.93263) | -1 | -1 |
| G: -5715.18379 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.54567 HOMO: -6.35114 LUMO: 1.92112 factor:1 | 1 (-2.99619) | -1 | -1 |
| G: -5715.18379 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.45035 HOMO: -6.53617 LUMO: 1.75241 factor:1 | 1 (-2.90087) | -1 | -1 |
| G: -5715.18379 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.60684 HOMO: -6.60420 LUMO: 1.78779 factor:1 | 1 (-3.05736) | -1 | -1 |
| G: -5715.18379 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.17806 HOMO: -7.40422 LUMO: -0.97145 factor:1 | 1 (-0.62858) | -1 | -1 |
| G: -5715.18379 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.06337 HOMO: -6.80013 LUMO: -0.69117 factor:1 | 1 (-0.51389) | -1 | -1 |
| G: -5715.18379 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.00359 HOMO: -6.68040 LUMO: -0.47076 factor:1 | 1 (-2.45411) | -1 | -1 |
| G: -5715.18379 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.11699 HOMO: -7.20285 LUMO: -0.66124 factor:1 | 1 (-1.56751) | -1 | -1 |
| G: -5715.18379 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.17620 HOMO: -6.82734 LUMO: -0.60137 factor:1 | 1 (-2.62672) | -1 | -1 |
| G: -5715.18379 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.48124 HOMO: -7.18653 LUMO: 0.59321 factor:1 | 1 (-1.93176) | -1 | -1 |
| G: -5715.18379 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.81039 HOMO: -7.29265 LUMO: 0.48164 factor:1 | 1 (-2.26091) | -1 | -1 |
| G: -5715.18379 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.25233 HOMO: -6.63414 LUMO: -0.25034 factor:1 | 1 (-2.70285) | -1 | -1 |
| G: -5715.18379 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.33716 HOMO: -7.20285 LUMO: 0.53879 factor:1 | 1 (-1.78768) | -1 | -1 |
| G: -5715.18379 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.54614 HOMO: -6.46815 LUMO: -0.21769 factor:1 | 1 (-1.99666) | -1 | -1 |
| G: -5715.18379 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.54640 HOMO: -6.57971 LUMO: -0.18776 factor:1 | 1 (-0.99692) | -1 | -1 |
| G: -5715.18379 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.06527 HOMO: -6.90897 LUMO: 1.91296 factor:1 | 1 (-0.51579) | -1 | -1 |
| G: -5715.18379 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.24786 HOMO: -6.67495 LUMO: 2.04358 factor:1 | 1 (-0.69838) | -1 | -1 |
| G: -5715.18379 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.59723 HOMO: -6.94162 LUMO: 1.73881 factor:1 | 1 (-1.04775) | -1 | -1 |
| G: -5715.18379 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.40740 HOMO: -6.73482 LUMO: 1.95922 factor:1 | 1 (-0.85792) | -1 | -1 |
| G: -5715.18379 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.96932 HOMO: -6.70489 LUMO: 2.04358 factor:1 | 1 (-1.41984) | -1 | -1 |
| G: -5715.18379 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.74863 HOMO: -7.04231 LUMO: 1.79323 factor:1 | 1 (-1.19915) | -1 | -1 |
| G: -5715.18379 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.92581 HOMO: -6.68584 LUMO: 1.60275 factor:1 | 1 (-1.37632) | -1 | -1 |
| G: -5715.18379 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.60169 HOMO: -6.40556 LUMO: 1.45581 factor:1 | 1 (-1.05221) | -1 | -1 |
| G: -5715.18379 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.16401 HOMO: -6.94979 LUMO: 2.16603 factor:1 | 1 (-1.61453) | -1 | -1 |
| G: -5715.18379 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.76912 HOMO: -6.84911 LUMO: 1.89935 factor:1 | 1 (-1.21964) | -1 | -1 |
| G: -5715.18379 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.40155 HOMO: -6.22052 LUMO: 1.57282 factor:1 | 1 (-0.85207) | -1 | -1 |
| G: -5715.18379 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11979.86826 HOMO: -6.51168 LUMO: 2.10072 factor:1 | 1 (-0.31878) | -1 | -1 |
| G: -5715.18379 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.35842 HOMO: -7.03686 LUMO: 2.12249 factor:1 | 1 (-0.80894) | -1 | -1 |
| G: -5715.18379 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11979.85248 HOMO: -6.84094 LUMO: 1.63268 factor:1 | 1 (-0.30300) | -1 | -1 |
| G: -5715.18379 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.00446 HOMO: -6.75387 LUMO: 1.72248 factor:1 | 1 (-0.45497) | -1 | -1 |
| G: -5715.18379 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.21317 HOMO: -6.86271 LUMO: 1.68711 factor:1 | 1 (-0.66369) | -1 | -1 |
| G: -5715.18379 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11979.80954 HOMO: -6.84094 LUMO: 2.02997 factor:1 | 1 (-0.26006) | -1 | -1 |
| G: -5715.18379 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11979.92533 HOMO: -6.80557 LUMO: 2.02725 factor:1 | 1 (-0.37584) | -1 | -1 |
| G: -5715.18379 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.23722 HOMO: -6.38651 LUMO: 1.53472 factor:1 | 1 (-0.68774) | -1 | -1 |
| G: -5715.18379 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11979.89803 HOMO: -7.51306 LUMO: 0.28572 factor:1 | 1 (-0.34855) | -1 | -1 |
| G: -5715.18379 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.82959 HOMO: -6.97972 LUMO: -0.74287 factor:1 | 1 (-1.28011) | -1 | -1 |
| G: -5715.18379 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.96543 HOMO: -6.83822 LUMO: -0.65852 factor:1 | 1 (-1.41594) | -1 | -1 |
| G: -5715.18379 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.52041 HOMO: -6.71305 LUMO: -0.49525 factor:1 | 1 (-0.97093) | -1 | -1 |
| G: -5715.18379 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.59268 HOMO: -6.60692 LUMO: -0.22313 factor:1 | 1 (-1.04320) | -1 | -1 |
| G: -5715.18379 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.20765 HOMO: -7.20013 LUMO: 0.55239 factor:1 | 1 (-2.65817) | -1 | -1 |
| G: -5715.18379 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.73686 HOMO: -6.60420 LUMO: -0.28028 factor:1 | 1 (-3.18738) | -1 | -1 |
| G: -5715.18379 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.16912 HOMO: -6.69128 LUMO: -0.30477 factor:1 | 1 (-2.61964) | -1 | -1 |
| G: -5715.18379 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.12441 HOMO: -6.65591 LUMO: -0.25579 factor:1 | 1 (-2.57493) | -1 | -1 |
| G: -5715.18379 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.34866 HOMO: -6.69128 LUMO: 1.70888 factor:1 | 1 (-2.79918) | -1 | -1 |
| G: -5715.18379 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.18346 HOMO: -6.50080 LUMO: 1.87759 factor:1 | 1 (-2.63398) | -1 | -1 |
| G: -5715.18379 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.43057 HOMO: -6.85727 LUMO: 1.99187 factor:1 | 1 (-2.88109) | -1 | -1 |
| G: -5715.18379 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.35489 HOMO: -6.58788 LUMO: 1.79051 factor:1 | 1 (-2.80541) | -1 | -1 |
| G: -5715.18379 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.83690 HOMO: -6.64230 LUMO: 2.16058 factor:1 | 1 (-2.28742) | -1 | -1 |
| G: -5715.18379 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.24251 HOMO: -6.58788 LUMO: 2.10616 factor:1 | 1 (-2.69303) | -1 | -1 |
| G: -5715.18379 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.20281 HOMO: -7.01782 LUMO: 2.13609 factor:1 | 1 (-2.65333) | -1 | -1 |
| G: -5715.18379 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11979.82674 HOMO: -6.31304 LUMO: 2.31841 factor:1 | 1 (-0.27726) | -1 | -1 |
| G: -5715.18379 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.46358 HOMO: -6.94979 LUMO: 2.07895 factor:1 | 1 (-1.91410) | -1 | -1 |
| G: -5715.18379 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.88357 HOMO: -6.88992 LUMO: 2.28031 factor:1 | 1 (-1.33409) | -1 | -1 |
| G: -5715.18379 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.05372 HOMO: -6.66407 LUMO: 2.07623 factor:1 | 1 (-2.50424) | -1 | -1 |
| G: -5715.18379 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.17920 HOMO: -6.52529 LUMO: 1.70071 factor:1 | 1 (-1.62972) | -1 | -1 |
| G: -5715.18379 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.32892 HOMO: -6.58788 LUMO: 1.57282 factor:1 | 1 (-1.77943) | -1 | -1 |
| G: -5715.18379 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.55826 HOMO: -6.55250 LUMO: 1.95378 factor:1 | 1 (-1.00878) | -1 | -1 |
| G: -5715.18379 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.89508 HOMO: -6.24773 LUMO: 1.77962 factor:1 | 1 (-2.34559) | -1 | -1 |
| G: -5715.18379 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.04491 HOMO: -6.31304 LUMO: 2.18507 factor:1 | 1 (-1.49543) | -1 | -1 |
| G: -5715.18379 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.28541 HOMO: -6.18243 LUMO: 2.01636 factor:1 | 1 (-0.73593) | -1 | -1 |
| G: -5715.18379 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.00726 HOMO: -6.99877 LUMO: 2.14970 factor:1 | 1 (-0.45778) | -1 | -1 |
| G: -5715.18379 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.41739 HOMO: -6.72665 LUMO: 2.07079 factor:1 | 1 (-0.86791) | -1 | -1 |
| G: -5715.18379 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.25504 HOMO: -6.36202 LUMO: 2.17419 factor:1 | 1 (-1.70556) | -1 | -1 |
| G: -5715.18379 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.86774 HOMO: -6.78652 LUMO: 2.05718 factor:1 | 1 (-1.31826) | -1 | -1 |
| G: -5715.18379 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.81707 HOMO: -6.87360 LUMO: 2.34290 factor:1 | 1 (-1.26759) | -1 | -1 |
| G: -5715.18379 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.57445 HOMO: -6.62053 LUMO: 1.89391 factor:1 | 1 (-1.02497) | -1 | -1 |
| G: -5715.18379 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.09841 HOMO: -6.58788 LUMO: 1.83133 factor:1 | 1 (-1.54893) | -1 | -1 |
| G: -5715.18379 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.36411 HOMO: -7.08584 LUMO: 1.91568 factor:1 | 1 (-0.81463) | 1 | 1 |
| G: -5715.18379 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.23709 HOMO: -6.56883 LUMO: 1.81228 factor:1 | 1 (-0.68760) | -1 | -1 |
| G: -5715.18379 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.16187 HOMO: -6.66135 LUMO: 1.92384 factor:1 | 1 (-0.61239) | -1 | -1 |
| G: -5715.18379 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.10478 HOMO: -6.64502 LUMO: 2.15786 factor:1 | 1 (-0.55530) | -1 | -1 |
| G: -5715.18379 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.31872 HOMO: -6.71305 LUMO: 1.91840 factor:1 | 1 (-0.76924) | -1 | -1 |
| G: -5715.18379 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.15710 HOMO: -6.44094 LUMO: 1.74425 factor:1 | 1 (-1.60762) | -1 | -1 |
| G: -5715.18379 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.52421 HOMO: -6.51985 LUMO: 1.84221 factor:1 | 1 (-1.97473) | -1 | -1 |
| G: -5715.18379 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.76760 HOMO: -6.63414 LUMO: -0.24762 factor:1 | 1 (-1.21812) | -1 | -1 |
| G: -5715.18379 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.22483 HOMO: -6.60420 LUMO: -0.22585 factor:1 | 1 (-1.67535) | -1 | -1 |
| G: -5715.18379 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.02524 HOMO: -7.19741 LUMO: 0.58232 factor:1 | 1 (-1.47576) | -1 | -1 |
| G: -5715.18379 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.36288 HOMO: -6.77019 LUMO: -0.56872 factor:1 | 1 (-1.81339) | -1 | -1 |
| G: -5715.18379 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.91389 HOMO: -7.46136 LUMO: 0.28844 factor:1 | 1 (-1.36441) | -1 | -1 |
| G: -5715.18379 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.40829 HOMO: -6.60420 LUMO: -0.54151 factor:1 | 1 (-1.85881) | -1 | -1 |
| G: -5715.18379 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.96420 HOMO: -6.53890 LUMO: -0.46531 factor:1 | 1 (-1.41472) | -1 | -1 |
| G: -5715.18379 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.59042 HOMO: -6.81645 LUMO: -0.57144 factor:1 | 1 (-2.04094) | -1 | -1 |
| G: -5715.18379 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.26048 HOMO: -7.48041 LUMO: 0.28572 factor:1 | 1 (-1.71100) | -1 | -1 |
| G: -5715.18379 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.63605 HOMO: -6.75659 LUMO: -0.45715 factor:1 | 1 (-2.08657) | -1 | -1 |
| G: -5715.18379 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.67651 HOMO: -6.66135 LUMO: -0.41906 factor:1 | 1 (-2.12703) | -1 | -1 |
| G: -5715.18379 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.36805 HOMO: -6.55794 LUMO: -0.27483 factor:1 | 1 (-1.81856) | -1 | -1 |
| G: -5715.18379 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.81331 HOMO: -7.07496 LUMO: -0.63403 factor:1 | 1 (-1.26383) | -1 | -1 |
| G: -5715.18379 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.75644 HOMO: -7.12394 LUMO: 0.53334 factor:1 | 1 (-1.20696) | -1 | -1 |
| G: -5715.18379 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.49386 HOMO: -6.53617 LUMO: -0.25579 factor:1 | 1 (-2.94438) | -1 | -1 |
| G: -5715.18379 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.26823 HOMO: -6.50896 LUMO: -0.25034 factor:1 | 1 (-2.71874) | -1 | -1 |
| G: -5715.18379 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.89508 HOMO: -7.17564 LUMO: -0.68573 factor:1 | 1 (-2.34559) | -1 | -1 |
| G: -5715.18379 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.13647 HOMO: -6.53617 LUMO: -0.30749 factor:1 | 1 (-2.58699) | -1 | -1 |
| G: -5715.18379 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.25125 HOMO: -6.55522 LUMO: -0.30749 factor:1 | 1 (-2.70176) | -1 | -1 |
| G: -5715.18379 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.22910 HOMO: -7.05591 LUMO: -0.71022 factor:1 | 1 (-2.67961) | -1 | -1 |
| G: -5715.18379 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.36779 HOMO: -7.17564 LUMO: -0.69933 factor:1 | 1 (-2.81831) | -1 | -1 |
| G: -5715.18379 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11983.06062 HOMO: -6.78380 LUMO: -0.67756 factor:1 | 1 (-3.51114) | -1 | -1 |
| G: -5715.18379 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.22752 HOMO: -6.62325 LUMO: 2.02725 factor:1 | 1 (-2.67804) | -1 | -1 |
| G: -5715.18379 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.81825 HOMO: -6.63414 LUMO: 1.91296 factor:1 | 1 (-3.26877) | -1 | -1 |
| G: -5715.18379 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11983.04797 HOMO: -6.83278 LUMO: 1.65717 factor:1 | 1 (-3.49849) | -1 | -1 |
| G: -5715.18379 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11983.17711 HOMO: -6.66407 LUMO: 1.95650 factor:1 | 1 (-3.62763) | -1 | -1 |
| G: -5715.18379 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.22319 HOMO: -6.61237 LUMO: 2.11432 factor:1 | 1 (-2.67371) | -1 | -1 |
| G: -5715.18379 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.37849 HOMO: -6.62053 LUMO: 2.09256 factor:1 | 1 (-2.82900) | -1 | -1 |
| G: -5715.18379 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.74102 HOMO: -6.78652 LUMO: 2.13609 factor:1 | 1 (-3.19154) | -1 | -1 |
| G: -5715.18379 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.86464 HOMO: -6.94707 LUMO: 1.81772 factor:1 | 1 (-3.31516) | -1 | -1 |
| G: -5715.18379 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11983.20443 HOMO: -6.85183 LUMO: 2.12793 factor:1 | 1 (-3.65495) | -1 | -1 |
| G: -5715.18379 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.92873 HOMO: -6.81101 LUMO: 1.83949 factor:1 | 1 (-3.37925) | -1 | -1 |
| G: -5715.18379 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.22496 HOMO: -6.98788 LUMO: 2.16058 factor:1 | 1 (-2.67548) | -1 | -1 |
| G: -5715.18379 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11983.08971 HOMO: -6.62869 LUMO: 2.00820 factor:1 | 1 (-3.54023) | -1 | -1 |
| G: -5715.18379 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.34243 HOMO: -6.34025 LUMO: 2.25855 factor:1 | 1 (-2.79295) | -1 | -1 |
| G: -5715.18379 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11983.23344 HOMO: -6.01372 LUMO: 2.01636 factor:1 | 1 (-3.68396) | -1 | -1 |
| G: -5715.18379 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.51740 HOMO: -6.89264 LUMO: 2.27487 factor:1 | 1 (-2.96792) | -1 | -1 |
| G: -5715.18379 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.34004 HOMO: -6.53073 LUMO: 2.20684 factor:1 | 1 (-2.79055) | -1 | -1 |
| G: -5715.18379 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.27138 HOMO: -6.83278 LUMO: 1.53744 factor:1 | 1 (-2.72190) | -1 | -1 |
| G: -5715.18379 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11983.08127 HOMO: -6.41917 LUMO: 1.82316 factor:1 | 1 (-3.53179) | -1 | -1 |
| G: -5715.18379 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11983.10685 HOMO: -6.56339 LUMO: 1.63813 factor:1 | 1 (-3.55737) | -1 | -1 |
| G: -5715.18379 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11983.39818 HOMO: -6.88992 LUMO: 1.65173 factor:1 | 1 (-3.84870) | -1 | -1 |
| G: -5715.18379 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.30591 HOMO: -6.63141 LUMO: 1.92112 factor:1 | 1 (-2.75643) | -1 | -1 |
| G: -5715.18379 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.35628 HOMO: -6.83822 LUMO: 1.88847 factor:1 | 1 (-2.80680) | -1 | -1 |
| G: -5715.18379 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.48502 HOMO: -6.84638 LUMO: 1.90480 factor:1 | 1 (-2.93554) | -1 | -1 |
| G: -5715.18379 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11983.33527 HOMO: -6.82462 LUMO: 1.70888 factor:1 | 1 (-3.78578) | -1 | -1 |
| G: -5715.18379 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11983.07738 HOMO: -6.82734 LUMO: 2.12521 factor:1 | 1 (-3.52790) | -1 | -1 |
| G: -5715.18379 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.93841 HOMO: -6.94435 LUMO: 1.87214 factor:1 | 1 (-3.38893) | -1 | -1 |
| G: -5715.18379 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.33299 HOMO: -6.98516 LUMO: 2.51433 factor:1 | 1 (-2.78351) | -1 | -1 |
| G: -5715.18379 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.74962 HOMO: -6.74026 LUMO: 2.15514 factor:1 | 1 (-3.20014) | -1 | -1 |
| G: -5715.18379 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.35345 HOMO: -6.93618 LUMO: 2.54426 factor:1 | 1 (-2.80397) | -1 | -1 |
| G: -5715.18379 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.16885 HOMO: -6.28583 LUMO: 2.53610 factor:1 | 1 (-2.61937) | -1 | -1 |
| G: -5715.18379 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.28689 HOMO: -6.56883 LUMO: 1.94834 factor:1 | 1 (-2.73741) | -1 | -1 |
| G: -5715.18379 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.32613 HOMO: -7.08584 LUMO: 1.99187 factor:1 | 1 (-2.77665) | 1 | 1 |
| G: -5715.18379 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11983.21129 HOMO: -6.19059 LUMO: 1.99732 factor:1 | 1 (-3.66181) | -1 | -1 |
| G: -5715.18379 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.42681 HOMO: -6.78108 LUMO: 2.03813 factor:1 | 1 (-2.87733) | -1 | -1 |
| G: -5715.18379 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.90307 HOMO: -6.82189 LUMO: 1.77418 factor:1 | 1 (-3.35359) | -1 | -1 |
| G: -5715.18379 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.48227 HOMO: -6.45454 LUMO: 1.78779 factor:1 | 1 (-2.93279) | -1 | -1 |
| G: -5715.18379 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11983.18533 HOMO: -6.84366 LUMO: 1.77690 factor:1 | 1 (-3.63585) | -1 | -1 |
| G: -5715.18379 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11983.32865 HOMO: -6.74026 LUMO: 1.67622 factor:1 | 1 (-3.77917) | -1 | -1 |
| G: -5715.18379 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.75087 HOMO: -6.76475 LUMO: 2.40277 factor:1 | 1 (-3.20139) | -1 | -1 |
| G: -5715.18379 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.16977 HOMO: -6.65863 LUMO: 1.86670 factor:1 | 1 (-2.62029) | -1 | -1 |
| G: -5715.18379 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.98340 HOMO: -6.50080 LUMO: 1.93201 factor:1 | 1 (-3.43391) | -1 | -1 |
| G: -5715.18379 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.35536 HOMO: -6.34842 LUMO: 1.70888 factor:1 | 1 (-2.80587) | -1 | -1 |
| G: -5715.18379 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.43032 HOMO: -6.60692 LUMO: 2.20140 factor:1 | 1 (-2.88084) | -1 | -1 |
| G: -5715.18379 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.15938 HOMO: -6.74026 LUMO: 2.14970 factor:1 | 1 (-2.60990) | -1 | -1 |
| G: -5715.18379 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.96533 HOMO: -6.63686 LUMO: 2.17419 factor:1 | 1 (-3.41585) | -1 | -1 |
| G: -5715.18379 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.94126 HOMO: -6.81917 LUMO: 2.10072 factor:1 | 1 (-1.39178) | -1 | -1 |
| G: -5715.18379 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.10401 HOMO: -6.92802 LUMO: 2.04358 factor:1 | 1 (-1.55453) | -1 | -1 |
| G: -5715.18379 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.75798 HOMO: -6.56067 LUMO: -0.47620 factor:1 | 1 (-2.20850) | -1 | -1 |
| G: -5715.18379 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.12984 HOMO: -6.56611 LUMO: -0.77008 factor:1 | 1 (-1.58036) | -1 | -1 |
| G: -5715.18379 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.29681 HOMO: -6.78380 LUMO: -0.64763 factor:1 | 1 (-1.74732) | -1 | -1 |
| G: -5715.18379 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.04958 HOMO: -6.51985 LUMO: -0.24490 factor:1 | 1 (-2.50010) | -1 | -1 |
| G: -5715.18379 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.90445 HOMO: -6.52529 LUMO: -0.27483 factor:1 | 1 (-3.35497) | -1 | -1 |
| G: -5715.18379 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11983.00590 HOMO: -7.10489 LUMO: -0.62586 factor:1 | 1 (-3.45642) | -1 | -1 |
| G: -5715.18379 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11983.07863 HOMO: -7.18108 LUMO: 0.48980 factor:1 | 1 (-3.52915) | -1 | -1 |
| G: -5715.18379 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11983.15235 HOMO: -7.14299 LUMO: -0.63947 factor:1 | 1 (-3.60287) | -1 | -1 |
| G: -5715.18379 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11983.19339 HOMO: -6.70761 LUMO: -0.54423 factor:1 | 1 (-3.64390) | -1 | -1 |
| G: -5715.18379 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11983.04165 HOMO: -7.32258 LUMO: -1.03675 factor:1 | 1 (-3.49217) | -1 | -1 |
| G: -5715.18379 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11983.09844 HOMO: -6.65046 LUMO: -0.41361 factor:1 | 1 (-3.54896) | -1 | -1 |
| G: -5715.18379 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.86124 HOMO: -6.76475 LUMO: -0.60137 factor:1 | 1 (-3.31176) | -1 | -1 |
| G: -5715.18379 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11983.08653 HOMO: -6.77836 LUMO: -0.54423 factor:1 | 1 (-3.53704) | -1 | -1 |
| G: -5715.18379 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.86706 HOMO: -7.52395 LUMO: 0.26395 factor:1 | 1 (-1.31758) | -1 | -1 |
| G: -5715.18379 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.03433 HOMO: -6.93890 LUMO: -0.72382 factor:1 | 1 (-1.48484) | -1 | -1 |
| G: -5715.18379 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.01892 HOMO: -6.72938 LUMO: -0.47348 factor:1 | 1 (-1.46944) | -1 | -1 |
| G: -5715.18379 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.84461 HOMO: -6.66951 LUMO: -0.40817 factor:1 | 1 (-1.29513) | -1 | -1 |
| G: -5715.18379 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.73139 HOMO: -6.60420 LUMO: -0.19320 factor:1 | 1 (-3.18191) | -1 | -1 |
| G: -5715.18379 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.85701 HOMO: -6.67495 LUMO: -0.27211 factor:1 | 1 (-2.30753) | -1 | -1 |
| G: -5715.18379 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.82992 HOMO: -7.23823 LUMO: -0.62858 factor:1 | 1 (-3.28044) | -1 | -1 |
| G: -5715.18379 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.74554 HOMO: -7.27088 LUMO: 0.53334 factor:1 | 1 (-3.19606) | -1 | -1 |
| G: -5715.18379 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.92841 HOMO: -7.20013 LUMO: 0.59049 factor:1 | 1 (-2.37893) | -1 | -1 |
| G: -5715.18379 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.28741 HOMO: -6.60148 LUMO: -0.20953 factor:1 | 1 (-2.73793) | -1 | -1 |
| G: -5715.18379 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.15835 HOMO: -6.69400 LUMO: -0.51974 factor:1 | 1 (-2.60886) | -1 | -1 |
| G: -5715.18379 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.80032 HOMO: -7.40422 LUMO: -0.98777 factor:1 | 1 (-3.25084) | -1 | -1 |
| G: -5715.18379 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.97810 HOMO: -6.88176 LUMO: -0.71022 factor:1 | 1 (-2.42862) | -1 | -1 |
| G: -5715.18379 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.70740 HOMO: -6.86271 LUMO: -0.59321 factor:1 | 1 (-2.15792) | -1 | -1 |
| G: -5715.18379 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.64851 HOMO: -6.73754 LUMO: -0.55239 factor:1 | 1 (-2.09903) | -1 | -1 |
| G: -5715.18379 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.39903 HOMO: -6.71033 LUMO: 1.57010 factor:1 | 1 (-2.84955) | -1 | -1 |
| G: -5715.18379 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.48611 HOMO: -6.69672 LUMO: 1.68711 factor:1 | 1 (-2.93663) | -1 | -1 |
| G: -5715.18379 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.53988 HOMO: -6.67495 LUMO: 2.03813 factor:1 | 1 (-2.99040) | -1 | -1 |
| G: -5715.18379 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.59174 HOMO: -6.54434 LUMO: 1.83677 factor:1 | 1 (-3.04226) | -1 | -1 |
| G: -5715.18379 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.46943 HOMO: -6.57155 LUMO: 1.77146 factor:1 | 1 (-2.91994) | -1 | -1 |
| G: -5715.18379 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.53811 HOMO: -6.76747 LUMO: 1.87759 factor:1 | 1 (-2.98863) | -1 | -1 |
| G: -5715.18379 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.31364 HOMO: -6.58243 LUMO: 1.61364 factor:1 | 1 (-2.76416) | -1 | -1 |
| G: -5715.18379 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.33492 HOMO: -6.61781 LUMO: 2.13881 factor:1 | 1 (-2.78544) | -1 | -1 |
| G: -5715.18379 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.30810 HOMO: -6.62597 LUMO: 2.00276 factor:1 | 1 (-1.75862) | -1 | -1 |
| G: -5715.18379 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.36449 HOMO: -7.01237 LUMO: 1.95922 factor:1 | 1 (-0.81501) | -1 | -1 |
| G: -5715.18379 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.35543 HOMO: -7.03959 LUMO: 2.16875 factor:1 | 1 (-0.80595) | -1 | -1 |
| G: -5715.18379 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.50011 HOMO: -6.83278 LUMO: 1.91296 factor:1 | 1 (-0.95063) | -1 | -1 |
| G: -5715.18379 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.16912 HOMO: -6.40012 LUMO: 1.95650 factor:1 | 1 (-2.61964) | -1 | -1 |
| G: -5715.18379 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.40723 HOMO: -6.50080 LUMO: 1.73337 factor:1 | 1 (-1.85775) | -1 | -1 |
| G: -5715.18379 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.05638 HOMO: -6.95795 LUMO: 2.28848 factor:1 | 1 (-2.50690) | -1 | -1 |
| G: -5715.18379 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.24369 HOMO: -6.63686 LUMO: 2.20140 factor:1 | 1 (-1.69421) | -1 | -1 |
| G: -5715.18379 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.41464 HOMO: -6.57427 LUMO: 1.87214 factor:1 | 1 (-0.86516) | -1 | -1 |
| G: -5715.18379 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.42523 HOMO: -6.38379 LUMO: 2.32113 factor:1 | 1 (-0.87574) | -1 | -1 |
| G: -5715.18379 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.44662 HOMO: -6.63958 LUMO: 2.04902 factor:1 | 1 (-2.89714) | -1 | -1 |
| G: -5715.18379 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.89890 HOMO: -6.70216 LUMO: 1.93201 factor:1 | 1 (-3.34942) | -1 | -1 |
| G: -5715.18379 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.17821 HOMO: -6.80557 LUMO: 2.23678 factor:1 | 1 (-2.62873) | -1 | -1 |
| G: -5715.18379 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.30257 HOMO: -6.72938 LUMO: 2.28304 factor:1 | 1 (-2.75308) | -1 | -1 |
| G: -5715.18379 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.36093 HOMO: -6.56067 LUMO: 1.66806 factor:1 | 1 (-2.81145) | -1 | -1 |
| G: -5715.18379 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.87458 HOMO: -6.95523 LUMO: 2.33474 factor:1 | 1 (-3.32510) | -1 | -1 |
| G: -5715.18379 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.31976 HOMO: -6.59876 LUMO: 2.30480 factor:1 | 1 (-2.77028) | -1 | -1 |
| G: -5715.18379 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.36191 HOMO: -6.87360 LUMO: 1.75786 factor:1 | 1 (-2.81243) | -1 | -1 |
| G: -5715.18379 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.17658 HOMO: -7.06408 LUMO: 1.99187 factor:1 | 1 (-2.62710) | 1 | 1 |
| G: -5715.18379 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.37737 HOMO: -6.95795 LUMO: 1.88847 factor:1 | 1 (-2.82789) | -1 | -1 |
| G: -5715.18379 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11979.97384 HOMO: -6.85455 LUMO: 1.63813 factor:1 | 1 (-0.42436) | -1 | -1 |
| G: -5715.18379 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11979.93188 HOMO: -7.09129 LUMO: 2.31569 factor:1 | 1 (-0.38240) | 1 | 1 |
| G: -5715.18379 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.99932 HOMO: -6.91441 LUMO: 1.68983 factor:1 | 1 (-2.44984) | -1 | -1 |
| G: -5715.18379 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.06556 HOMO: -6.89809 LUMO: 2.23678 factor:1 | 1 (-1.51608) | -1 | -1 |
| G: -5715.18379 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.94700 HOMO: -6.78652 LUMO: 1.98371 factor:1 | 1 (-2.39751) | -1 | -1 |
| G: -5715.18379 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.09038 HOMO: -6.94707 LUMO: 2.23678 factor:1 | 1 (-1.54090) | -1 | -1 |
| G: -5715.18379 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.03457 HOMO: -7.07224 LUMO: 2.13337 factor:1 | 1 (-1.48509) | 1 | 1 |
| G: -5715.18379 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.99910 HOMO: -6.94979 LUMO: 2.28031 factor:1 | 1 (-2.44962) | -1 | -1 |
| G: -5715.18379 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.13588 HOMO: -6.60965 LUMO: 2.20412 factor:1 | 1 (-1.58640) | -1 | -1 |
| G: -5715.18379 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.86249 HOMO: -6.87360 LUMO: 2.40277 factor:1 | 1 (-1.31300) | -1 | -1 |
| G: -5715.18379 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.26328 HOMO: -6.92802 LUMO: 1.89663 factor:1 | 1 (-1.71380) | -1 | -1 |
| G: -5715.18379 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.07438 HOMO: -6.88448 LUMO: 2.02725 factor:1 | 1 (-1.52490) | -1 | -1 |
| G: -5715.18379 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.83506 HOMO: -6.69128 LUMO: 1.55105 factor:1 | 1 (-1.28557) | -1 | -1 |
| G: -5715.18379 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.11631 HOMO: -6.54978 LUMO: 1.93201 factor:1 | 1 (-1.56683) | -1 | -1 |
| G: -5715.18379 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.36671 HOMO: -6.19331 LUMO: 1.46941 factor:1 | 1 (-1.81723) | -1 | -1 |
| G: -5715.18379 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.90959 HOMO: -6.55794 LUMO: 1.89663 factor:1 | 1 (-1.36011) | -1 | -1 |
| G: -5715.18379 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.94575 HOMO: -6.07630 LUMO: 1.94289 factor:1 | 1 (-1.39627) | -1 | -1 |
| G: -5715.18379 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.00161 HOMO: -7.46408 LUMO: 0.31565 factor:1 | 1 (-2.45213) | -1 | -1 |
| G: -5715.18379 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.79333 HOMO: -6.63958 LUMO: -0.61770 factor:1 | 1 (-2.24385) | -1 | -1 |
| G: -5715.18379 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.12558 HOMO: -6.81101 LUMO: -0.57960 factor:1 | 1 (-2.57610) | -1 | -1 |
| G: -5715.18379 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.66492 HOMO: -6.74298 LUMO: -0.57960 factor:1 | 1 (-2.11544) | -1 | -1 |
| G: -5715.18379 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.77358 HOMO: -6.63686 LUMO: -0.42994 factor:1 | 1 (-2.22410) | -1 | -1 |
| G: -5715.18379 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.78076 HOMO: -6.60965 LUMO: -0.41089 factor:1 | 1 (-2.23128) | -1 | -1 |
| G: -5715.18379 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11983.07317 HOMO: -6.60692 LUMO: -0.80274 factor:1 | 1 (-3.52368) | -1 | -1 |
| G: -5715.18379 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.24950 HOMO: -6.58788 LUMO: -0.78097 factor:1 | 1 (-2.70002) | -1 | -1 |
| G: -5715.18379 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.28828 HOMO: -6.67767 LUMO: -0.48436 factor:1 | 1 (-2.73880) | -1 | -1 |
| G: -5715.18379 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11983.06051 HOMO: -6.63141 LUMO: -0.40545 factor:1 | 1 (-3.51103) | -1 | -1 |
| G: -5715.18379 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.25212 HOMO: -6.62053 LUMO: -0.83811 factor:1 | 1 (-2.70263) | -1 | -1 |
| G: -5715.18379 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11983.16495 HOMO: -6.59604 LUMO: -0.35375 factor:1 | 1 (-3.61547) | -1 | -1 |
| G: -5715.18379 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.11824 HOMO: -6.34297 LUMO: -0.39729 factor:1 | 1 (-2.56875) | -1 | -1 |
| G: -5715.18379 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.66848 HOMO: -6.67223 LUMO: 1.97827 factor:1 | 1 (-3.11900) | -1 | -1 |
| G: -5715.18379 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.49294 HOMO: -6.40012 LUMO: 1.89935 factor:1 | 1 (-2.94346) | -1 | -1 |
| G: -5715.18379 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.26771 HOMO: -6.74842 LUMO: 1.97283 factor:1 | 1 (-2.71823) | -1 | -1 |
| G: -5715.18379 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.27723 HOMO: -6.76747 LUMO: 2.17147 factor:1 | 1 (-2.72775) | -1 | -1 |
| G: -5715.18379 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.73683 HOMO: -6.72121 LUMO: 1.55649 factor:1 | 1 (-3.18735) | -1 | -1 |
| G: -5715.18379 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11983.12944 HOMO: -6.97700 LUMO: 2.04085 factor:1 | 1 (-3.57996) | -1 | -1 |
| G: -5715.18379 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.98645 HOMO: -7.06680 LUMO: 2.04085 factor:1 | 1 (-2.43697) | 1 | 1 |
| G: -5715.18379 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.89630 HOMO: -7.09673 LUMO: 2.35106 factor:1 | 1 (-2.34682) | 1 | 1 |
| G: -5715.18379 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.55977 HOMO: -6.83006 LUMO: 2.14970 factor:1 | 1 (-3.01029) | -1 | -1 |
| G: -5715.18379 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11983.13036 HOMO: -6.72665 LUMO: 2.20140 factor:1 | 1 (-3.58088) | -1 | -1 |
| G: -5715.18379 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.84081 HOMO: -6.77291 LUMO: 2.34562 factor:1 | 1 (-3.29133) | -1 | -1 |
| G: -5715.18379 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.61362 HOMO: -6.73754 LUMO: 2.00276 factor:1 | 1 (-3.06414) | -1 | -1 |
| G: -5715.18379 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.95470 HOMO: -7.04231 LUMO: 1.92112 factor:1 | 1 (-2.40521) | -1 | -1 |
| G: -5715.18379 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.49471 HOMO: -6.83822 LUMO: 1.72248 factor:1 | 1 (-2.94522) | -1 | -1 |
| G: -5715.18379 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.06749 HOMO: -6.57971 LUMO: 2.16603 factor:1 | 1 (-2.51801) | -1 | -1 |
| G: -5715.18379 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.75271 HOMO: -6.80013 LUMO: 1.88575 factor:1 | 1 (-2.20322) | -1 | -1 |
| G: -5715.18379 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.89260 HOMO: -6.93618 LUMO: 2.18235 factor:1 | 1 (-2.34312) | -1 | -1 |
| G: -5715.18379 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.07228 HOMO: -6.54706 LUMO: 1.91024 factor:1 | 1 (-2.52279) | -1 | -1 |
| G: -5715.18379 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.84441 HOMO: -7.06952 LUMO: 2.18507 factor:1 | 1 (-2.29493) | 1 | 1 |
| G: -5715.18379 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.92451 HOMO: -7.05047 LUMO: 1.82044 factor:1 | 1 (-3.37503) | -1 | -1 |
| G: -5715.18379 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.93458 HOMO: -6.87632 LUMO: 1.92657 factor:1 | 1 (-3.38510) | -1 | -1 |
| G: -5715.18379 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.91614 HOMO: -6.58788 LUMO: 1.91568 factor:1 | 1 (-2.36666) | -1 | -1 |
| G: -5715.18379 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.03554 HOMO: -7.17292 LUMO: 1.90752 factor:1 | 1 (-2.48606) | 1 | 1 |
| G: -5715.18379 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.17739 HOMO: -6.93890 LUMO: 1.80684 factor:1 | 1 (-2.62791) | -1 | -1 |
| G: -5715.18379 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.37579 HOMO: -7.10761 LUMO: 2.20956 factor:1 | 1 (-2.82631) | 1 | 1 |
| G: -5715.18379 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.79512 HOMO: -6.85727 LUMO: 2.13609 factor:1 | 1 (-3.24564) | -1 | -1 |
| G: -5715.18379 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11983.04889 HOMO: -6.64502 LUMO: 1.38506 factor:1 | 1 (-3.49941) | -1 | -1 |
| G: -5715.18379 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.70402 HOMO: -6.87360 LUMO: 1.15648 factor:1 | 1 (-3.15453) | -1 | -1 |
| G: -5715.18379 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.77265 HOMO: -6.67223 LUMO: 2.07351 factor:1 | 1 (-2.22317) | -1 | -1 |
| G: -5715.18379 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.64288 HOMO: -6.29671 LUMO: 2.43270 factor:1 | 1 (-2.09340) | -1 | -1 |
| G: -5715.18379 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.82334 HOMO: -6.90897 LUMO: 2.28848 factor:1 | 1 (-3.27386) | -1 | -1 |
| G: -5715.18379 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11983.04282 HOMO: -7.04231 LUMO: 1.70071 factor:1 | 1 (-3.49334) | -1 | -1 |
| G: -5715.18379 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11983.01303 HOMO: -6.69944 LUMO: 1.94834 factor:1 | 1 (-3.46355) | -1 | -1 |
| G: -5715.18379 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.93980 HOMO: -6.56067 LUMO: 2.20956 factor:1 | 1 (-3.39032) | -1 | -1 |
| G: -5715.18379 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.86715 HOMO: -6.65046 LUMO: 2.06807 factor:1 | 1 (-3.31767) | -1 | -1 |
| G: -5715.18379 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11983.01706 HOMO: -7.08584 LUMO: 1.98915 factor:1 | 1 (-3.46757) | 1 | 1 |
| G: -5715.18379 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.95771 HOMO: -6.69400 LUMO: 2.09256 factor:1 | 1 (-3.40823) | -1 | -1 |
| G: -5715.18379 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.81920 HOMO: -6.62869 LUMO: 2.16331 factor:1 | 1 (-3.26972) | -1 | -1 |
| G: -5715.18379 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11983.24035 HOMO: -6.85183 LUMO: 2.16058 factor:1 | 1 (-3.69087) | -1 | -1 |
| G: -5715.18379 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11983.11110 HOMO: -6.54706 LUMO: 1.92384 factor:1 | 1 (-3.56162) | -1 | -1 |
| G: -5715.18379 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.92978 HOMO: -6.84366 LUMO: 2.48984 factor:1 | 1 (-1.38030) | -1 | -1 |
| G: -5715.18379 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.87748 HOMO: -6.77291 LUMO: 2.46263 factor:1 | 1 (-1.32800) | -1 | -1 |
| G: -5715.18379 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.71111 HOMO: -7.01782 LUMO: 2.31025 factor:1 | 1 (-1.16163) | -1 | -1 |
| G: -5715.18379 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.61315 HOMO: -6.94707 LUMO: 2.29664 factor:1 | 1 (-1.06367) | -1 | -1 |
| G: -5715.18379 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.15103 HOMO: -6.64230 LUMO: 1.97283 factor:1 | 1 (-2.60154) | -1 | -1 |
| G: -5715.18379 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.60309 HOMO: -6.47359 LUMO: 2.20412 factor:1 | 1 (-3.05361) | -1 | -1 |
| G: -5715.18379 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.79287 HOMO: -6.90625 LUMO: 1.92384 factor:1 | 1 (-2.24339) | -1 | -1 |
| G: -5715.18379 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.73547 HOMO: -7.17020 LUMO: 2.06807 factor:1 | 1 (-3.18599) | 1 | 1 |
| G: -5715.18379 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.88103 HOMO: -6.65046 LUMO: 2.20956 factor:1 | 1 (-2.33155) | -1 | -1 |
| G: -5715.18379 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.84154 HOMO: -7.07496 LUMO: 1.82861 factor:1 | 1 (-3.29206) | 1 | 1 |
| G: -5715.18379 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.01437 HOMO: -6.83006 LUMO: 2.14970 factor:1 | 1 (-2.46489) | -1 | -1 |
| G: -5715.18379 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.97032 HOMO: -6.92802 LUMO: 1.99187 factor:1 | 1 (-1.42084) | -1 | -1 |
| G: -5715.18379 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.91770 HOMO: -6.69672 LUMO: 2.36739 factor:1 | 1 (-1.36822) | -1 | -1 |
| G: -5715.18379 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.10614 HOMO: -7.13755 LUMO: 2.00276 factor:1 | 1 (-1.55665) | 1 | 1 |
| G: -5715.18379 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.53315 HOMO: -6.92530 LUMO: 2.25582 factor:1 | 1 (-0.98366) | -1 | -1 |
| G: -5715.18379 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11980.76605 HOMO: -6.77564 LUMO: 1.97827 factor:1 | 1 (-1.21657) | -1 | -1 |
| G: -5715.18379 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11982.27266 HOMO: -6.87904 LUMO: 1.60003 factor:1 | 1 (-2.72318) | -1 | -1 |
| G: -5715.18379 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.77137 HOMO: -6.62869 LUMO: 1.90480 factor:1 | 1 (-2.22189) | -1 | -1 |
| G: -5715.18379 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.90055 HOMO: -6.71033 LUMO: 1.54833 factor:1 | 1 (-2.35106) | -1 | -1 |
| G: -5715.18379 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.69262 HOMO: -6.74298 LUMO: 1.47486 factor:1 | 1 (-2.14314) | -1 | -1 |
| G: -5715.18379 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.45055 HOMO: -6.77019 LUMO: 1.90480 factor:1 | 1 (-1.90107) | -1 | -1 |
| G: -5715.18379 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11981.49305 HOMO: -6.70489 LUMO: 1.99459 factor:1 | 1 (-1.94357) | -1 | -1 |