乙二醇作为反应物的反应表19-1

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: -2104.18652 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -4185.45180 HOMO: -6.91169 LUMO: -0.53879 factor:2 | 1 (-2.35139) | -1 | -1 |
| G: -2104.18652 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -4184.20345 HOMO: -7.29809 LUMO: 2.83543 factor:2 | -1 (0.14531) | 1 | -1 |
| G: -2104.18652 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -8370.59048 HOMO: -6.86543 LUMO: -0.70205 factor:1 | 1 (-2.03827) | -1 | -1 |
| G: -2104.18652 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -8371.14783 HOMO: -7.47769 LUMO: 0.31293 factor:1 | 1 (-2.59561) | -1 | -1 |
| G: -2104.18652 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -8370.47625 HOMO: -6.63141 LUMO: -0.55511 factor:1 | 1 (-1.92404) | -1 | -1 |
| G: -2104.18652 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -8370.72317 HOMO: -6.68856 LUMO: -0.30205 factor:1 | 1 (-2.17095) | -1 | -1 |
| G: -2104.18652 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -8371.50332 HOMO: -7.22190 LUMO: 0.53334 factor:1 | 1 (-2.95110) | -1 | -1 |
| G: -2104.18652 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -8370.34474 HOMO: -6.66407 LUMO: -0.27756 factor:1 | 1 (-1.79252) | -1 | -1 |
| G: -2104.18652 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -8370.90322 HOMO: -7.15659 LUMO: -0.70205 factor:1 | 1 (-2.35101) | -1 | -1 |
| G: -2104.18652 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -8369.52714 HOMO: -6.69400 LUMO: 1.67622 factor:1 | 1 (-0.97493) | -1 | -1 |
| G: -2104.18652 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -8369.56725 HOMO: -6.60420 LUMO: 2.16058 factor:1 | 1 (-1.01504) | -1 | -1 |
| G: -2104.18652 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -8369.62924 HOMO: -6.87087 LUMO: 1.88031 factor:1 | 1 (-1.07703) | -1 | -1 |
| G: -2104.18652 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -8370.56061 HOMO: -6.60965 LUMO: -0.19864 factor:1 | 1 (-2.00839) | -1 | -1 |
| G: -2104.18652 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -8371.37605 HOMO: -7.29265 LUMO: 0.52246 factor:1 | 1 (-2.82383) | -1 | -1 |
| G: -2104.18652 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -8370.39113 HOMO: -6.86543 LUMO: -0.59593 factor:1 | 1 (-1.83892) | -1 | -1 |
| G: -2104.18652 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -8370.56858 HOMO: -7.44504 LUMO: -1.01226 factor:1 | 1 (-2.01636) | -1 | -1 |
| G: -2104.18652 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -8370.17295 HOMO: -6.92530 LUMO: -0.75103 factor:1 | 1 (-1.62074) | -1 | -1 |
| G: -2104.18652 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -8369.56421 HOMO: -7.10489 LUMO: 2.20412 factor:1 | 1 (-1.01199) | 1 | 1 |
| G: -2104.18652 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -8369.51898 HOMO: -6.58788 LUMO: 1.73881 factor:1 | 1 (-0.96677) | -1 | -1 |
| G: -2104.18652 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -8369.54919 HOMO: -6.64502 LUMO: 1.70343 factor:1 | 1 (-0.99697) | -1 | -1 |
| G: -2104.18652 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -8369.67779 HOMO: -6.73754 LUMO: 1.60819 factor:1 | 1 (-1.12557) | -1 | -1 |
| G: -2104.18652 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -8370.20044 HOMO: -6.80829 LUMO: 2.45991 factor:1 | 1 (-1.64822) | -1 | -1 |
| G: -2104.18652 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -8370.32245 HOMO: -6.91713 LUMO: 2.43814 factor:1 | 1 (-1.77024) | -1 | -1 |
| G: -2104.18652 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -8370.10963 HOMO: -6.60692 LUMO: 1.93745 factor:1 | 1 (-1.55742) | -1 | -1 |
| G: -2104.18652 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -8369.43269 HOMO: -6.26134 LUMO: 1.46125 factor:1 | 1 (-0.88048) | -1 | -1 |
| G: -2104.18652 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -8370.99270 HOMO: -7.54028 LUMO: 0.25851 factor:1 | 1 (-2.44048) | -1 | -1 |
| G: -2104.18652 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -8370.20882 HOMO: -6.97700 LUMO: -0.73471 factor:1 | 1 (-1.65660) | -1 | -1 |
| G: -2104.18652 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -8370.10389 HOMO: -6.92258 LUMO: -0.70205 factor:1 | 1 (-1.55167) | -1 | -1 |
| G: -2104.18652 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -8370.33214 HOMO: -6.83550 LUMO: -0.56872 factor:1 | 1 (-1.77992) | -1 | -1 |
| G: -2104.18652 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -8369.10518 HOMO: -6.72121 LUMO: 1.89663 factor:1 | 1 (-0.55296) | -1 | -1 |
| G: -2104.18652 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -8369.46355 HOMO: -6.73482 LUMO: 1.89935 factor:1 | 1 (-0.91134) | -1 | -1 |
| G: -2104.18652 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -8369.27168 HOMO: -6.61781 LUMO: 1.86670 factor:1 | 1 (-0.71947) | -1 | -1 |
| G: -2104.18652 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -8369.07173 HOMO: -7.01782 LUMO: 2.26399 factor:1 | 1 (-0.51952) | -1 | -1 |
| G: -2104.18652 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -8369.33397 HOMO: -7.23551 LUMO: 2.09800 factor:1 | 1 (-0.78176) | 1 | 1 |
| G: -2104.18652 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -8369.51041 HOMO: -7.13483 LUMO: 2.17963 factor:1 | 1 (-0.95819) | 1 | 1 |
| G: -2104.18652 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -8369.11625 HOMO: -6.22869 LUMO: 2.01092 factor:1 | 1 (-0.56404) | -1 | -1 |
| G: -2104.18652 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -8369.33653 HOMO: -6.80285 LUMO: 2.14970 factor:1 | 1 (-0.78431) | -1 | -1 |
| G: -2104.18652 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -8369.54913 HOMO: -7.21102 LUMO: 2.33746 factor:1 | 1 (-0.99692) | 1 | 1 |
| G: -2104.18652 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -8369.92617 HOMO: -6.39740 LUMO: 2.59597 factor:1 | 1 (-1.37396) | -1 | -1 |
| G: -2104.18652 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -8370.14419 HOMO: -7.07768 LUMO: 2.48168 factor:1 | 1 (-1.59197) | 1 | 1 |
| G: -2104.18652 HOMO: -7.74164 LUMO: 1.37690 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10474.68620 HOMO: -7.11306 LUMO: 0.90614 factor:1 | 1 (-1.94746) | -1 | -1 |
| G: -2104.18652 HOMO: -7.74164 LUMO: 1.37690 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10476.26756 HOMO: -6.61781 LUMO: -2.46263 factor:1 | 1 (-3.52883) | -1 | -1 |
| G: -2104.18652 HOMO: -7.74164 LUMO: 1.37690 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10474.76585 HOMO: -6.96611 LUMO: 0.90614 factor:1 | 1 (-2.02711) | -1 | -1 |
| G: -2104.18652 HOMO: -7.74164 LUMO: 1.37690 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10476.35020 HOMO: -6.86271 LUMO: -1.14832 factor:1 | 1 (-3.61147) | -1 | -1 |
| G: -2104.18652 HOMO: -7.74164 LUMO: 1.37690 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10475.05369 HOMO: -6.72665 LUMO: 0.96873 factor:1 | 1 (-2.31495) | -1 | -1 |
| G: -2104.18652 HOMO: -7.74164 LUMO: 1.37690 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10474.79717 HOMO: -7.14571 LUMO: 1.05036 factor:1 | 1 (-2.05843) | -1 | -1 |
| G: -2104.18652 HOMO: -7.74164 LUMO: 1.37690 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10474.52065 HOMO: -7.14299 LUMO: 0.98777 factor:1 | 1 (-1.78191) | -1 | -1 |
| G: -2104.18652 HOMO: -7.74164 LUMO: 1.37690 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10474.37177 HOMO: -6.99333 LUMO: 1.05852 factor:1 | 1 (-1.63304) | -1 | -1 |
| G: -2104.18652 HOMO: -7.74164 LUMO: 1.37690 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10476.71056 HOMO: -6.78924 LUMO: -1.49935 factor:1 | 1 (-3.97183) | -1 | -1 |
| G: -2104.18652 HOMO: -7.74164 LUMO: 1.37690 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10474.64772 HOMO: -7.13755 LUMO: 0.94151 factor:1 | 1 (-1.90899) | -1 | -1 |
| G: -2104.18652 HOMO: -7.74164 LUMO: 1.37690 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10477.16086 HOMO: -6.72938 LUMO: -0.35375 factor:1 | 1 (-4.42212) | -1 | -1 |
| G: -2104.18652 HOMO: -7.74164 LUMO: 1.37690 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10474.85703 HOMO: -6.99061 LUMO: 0.82450 factor:1 | 1 (-2.11830) | -1 | -1 |
| G: -2104.18652 HOMO: -7.74164 LUMO: 1.37690 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10475.97607 HOMO: -6.75114 LUMO: -0.68028 factor:1 | 1 (-3.23734) | -1 | -1 |
| G: -2104.18652 HOMO: -7.74164 LUMO: 1.37690 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10476.07823 HOMO: -6.40556 LUMO: -0.42722 factor:1 | 1 (-3.33949) | -1 | -1 |
| G: -2104.18652 HOMO: -7.74164 LUMO: 1.37690 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10476.96189 HOMO: -7.18653 LUMO: 0.42178 factor:1 | 1 (-4.22315) | -1 | -1 |
| G: -2104.18652 HOMO: -7.74164 LUMO: 1.37690 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10475.94660 HOMO: -6.63958 LUMO: -0.71294 factor:1 | 1 (-3.20787) | -1 | -1 |
| G: -2104.18652 HOMO: -7.74164 LUMO: 1.37690 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10476.07602 HOMO: -6.63958 LUMO: -0.71022 factor:1 | 1 (-3.33729) | -1 | -1 |
| G: -2104.18652 HOMO: -7.74164 LUMO: 1.37690 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10476.12800 HOMO: -6.69672 LUMO: -0.72654 factor:1 | 1 (-3.38926) | -1 | -1 |
| G: -2104.18652 HOMO: -7.74164 LUMO: 1.37690 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10475.74551 HOMO: -6.56883 LUMO: -0.80274 factor:1 | 1 (-3.00678) | -1 | -1 |
| G: -2104.18652 HOMO: -7.74164 LUMO: 1.37690 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10475.75961 HOMO: -6.68584 LUMO: -0.56872 factor:1 | 1 (-3.02087) | -1 | -1 |
| G: -2104.18652 HOMO: -7.74164 LUMO: 1.37690 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10476.04857 HOMO: -6.59060 LUMO: -0.35647 factor:1 | 1 (-3.30983) | -1 | -1 |
| G: -2104.18652 HOMO: -7.74164 LUMO: 1.37690 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10475.99082 HOMO: -6.72121 LUMO: -0.71838 factor:1 | 1 (-3.25209) | -1 | -1 |
| G: -2104.18652 HOMO: -7.74164 LUMO: 1.37690 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10476.58648 HOMO: -6.57971 LUMO: -0.61498 factor:1 | 1 (-3.84774) | -1 | -1 |
| G: -2104.18652 HOMO: -7.74164 LUMO: 1.37690 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10477.46816 HOMO: -7.07496 LUMO: 0.50613 factor:1 | 1 (-4.72942) | -1 | -1 |
| G: -2104.18652 HOMO: -7.74164 LUMO: 1.37690 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10477.25289 HOMO: -7.14027 LUMO: 0.43266 factor:1 | 1 (-4.51415) | -1 | -1 |
| G: -2104.18652 HOMO: -7.74164 LUMO: 1.37690 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10476.72466 HOMO: -6.43277 LUMO: -0.44082 factor:1 | 1 (-3.98592) | -1 | -1 |
| G: -2104.18652 HOMO: -7.74164 LUMO: 1.37690 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10475.85607 HOMO: -6.79468 LUMO: 0.07619 factor:1 | 1 (-3.11734) | -1 | -1 |
| G: -2104.18652 HOMO: -7.74164 LUMO: 1.37690 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10476.52958 HOMO: -6.81917 LUMO: -2.57148 factor:1 | 1 (-3.79085) | -1 | -1 |
| G: -2104.18652 HOMO: -7.74164 LUMO: 1.37690 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10474.66313 HOMO: -6.71849 LUMO: 1.30615 factor:1 | 1 (-1.92439) | -1 | -1 |
| G: -2104.18652 HOMO: -7.74164 LUMO: 1.37690 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10476.83002 HOMO: -6.85455 LUMO: -0.63675 factor:1 | 1 (-4.09129) | -1 | -1 |
| G: -2104.18652 HOMO: -7.74164 LUMO: 1.37690 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10476.98241 HOMO: -6.73210 LUMO: -1.03131 factor:1 | 1 (-4.24367) | -1 | -1 |
| G: -2104.18652 HOMO: -7.74164 LUMO: 1.37690 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10475.65479 HOMO: -6.83550 LUMO: -0.58777 factor:1 | 1 (-2.91605) | -1 | -1 |
| G: -2104.18652 HOMO: -7.74164 LUMO: 1.37690 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10475.78772 HOMO: -6.53073 LUMO: -0.74287 factor:1 | 1 (-3.04898) | -1 | -1 |
| G: -2104.18652 HOMO: -7.74164 LUMO: 1.37690 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10475.84951 HOMO: -7.18381 LUMO: -0.92791 factor:1 | 1 (-3.11078) | -1 | -1 |
| G: -2104.18652 HOMO: -7.74164 LUMO: 1.37690 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10475.86998 HOMO: -6.49264 LUMO: -0.44627 factor:1 | 1 (-3.13124) | -1 | -1 |
| G: -2104.18652 HOMO: -7.74164 LUMO: 1.37690 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10476.90412 HOMO: -7.32803 LUMO: 0.41361 factor:1 | 1 (-4.16538) | -1 | -1 |
| G: -2104.18652 HOMO: -7.74164 LUMO: 1.37690 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10476.01259 HOMO: -6.53073 LUMO: -0.52790 factor:1 | 1 (-3.27386) | -1 | -1 |
| G: -2104.18652 HOMO: -7.74164 LUMO: 1.37690 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10475.71400 HOMO: -6.54978 LUMO: -0.53062 factor:1 | 1 (-2.97527) | -1 | -1 |
| G: -2104.18652 HOMO: -7.74164 LUMO: 1.37690 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10475.87066 HOMO: -6.56611 LUMO: -0.37824 factor:1 | 1 (-3.13192) | -1 | -1 |
| G: -2104.18652 HOMO: -7.74164 LUMO: 1.37690 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10475.96353 HOMO: -6.57155 LUMO: -0.64219 factor:1 | 1 (-3.22479) | -1 | -1 |
| G: -2104.18652 HOMO: -7.74164 LUMO: 1.37690 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10476.51040 HOMO: -7.08040 LUMO: 0.45715 factor:1 | 1 (-3.77166) | -1 | -1 |
| G: -2104.18652 HOMO: -7.74164 LUMO: 1.37690 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10475.71958 HOMO: -6.66679 LUMO: -0.75376 factor:1 | 1 (-2.98084) | -1 | -1 |
| G: -2104.18652 HOMO: -7.74164 LUMO: 1.37690 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10475.74619 HOMO: -6.83550 LUMO: -0.99322 factor:1 | 1 (-3.00746) | -1 | -1 |
| G: -2104.18652 HOMO: -7.74164 LUMO: 1.37690 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10475.74924 HOMO: -6.53345 LUMO: -0.29660 factor:1 | 1 (-3.01050) | -1 | -1 |
| G: -2104.18652 HOMO: -7.74164 LUMO: 1.37690 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10474.34453 HOMO: -6.65046 LUMO: 2.40549 factor:1 | 1 (-1.60580) | -1 | -1 |
| G: -2104.18652 HOMO: -7.74164 LUMO: 1.37690 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10474.42383 HOMO: -6.98788 LUMO: 2.01092 factor:1 | 1 (-1.68509) | -1 | -1 |
| G: -2104.18652 HOMO: -7.74164 LUMO: 1.37690 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10474.28674 HOMO: -6.61781 LUMO: 1.92384 factor:1 | 1 (-1.54800) | -1 | -1 |
| G: -2104.18652 HOMO: -7.74164 LUMO: 1.37690 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10474.71064 HOMO: -6.61237 LUMO: 2.06807 factor:1 | 1 (-1.97190) | -1 | -1 |
| G: -2104.18652 HOMO: -7.74164 LUMO: 1.37690 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10474.79135 HOMO: -6.59060 LUMO: 1.95106 factor:1 | 1 (-2.05261) | -1 | -1 |
| G: -2104.18652 HOMO: -7.74164 LUMO: 1.37690 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10475.17181 HOMO: -6.48175 LUMO: 1.72248 factor:1 | 1 (-2.43308) | -1 | -1 |
| G: -2104.18652 HOMO: -7.74164 LUMO: 1.37690 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10475.36219 HOMO: -6.84911 LUMO: 2.03541 factor:1 | 1 (-2.62345) | -1 | -1 |
| G: -2104.18652 HOMO: -7.74164 LUMO: 1.37690 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10473.98967 HOMO: -6.50624 LUMO: 2.17147 factor:1 | 1 (-1.25093) | -1 | -1 |
| G: -2104.18652 HOMO: -7.74164 LUMO: 1.37690 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10474.01911 HOMO: -6.68312 LUMO: 2.08439 factor:1 | 1 (-1.28038) | -1 | -1 |
| G: -2104.18652 HOMO: -7.74164 LUMO: 1.37690 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10474.14646 HOMO: -6.96067 LUMO: 1.98099 factor:1 | 1 (-1.40773) | -1 | -1 |
| G: -2104.18652 HOMO: -7.74164 LUMO: 1.37690 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10474.80139 HOMO: -6.93618 LUMO: 1.85854 factor:1 | 1 (-2.06265) | -1 | -1 |
| G: -2104.18652 HOMO: -7.74164 LUMO: 1.37690 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10476.76188 HOMO: -6.71305 LUMO: -0.61226 factor:1 | 1 (-4.02315) | -1 | -1 |
| G: -2104.18652 HOMO: -7.74164 LUMO: 1.37690 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10474.31068 HOMO: -7.06408 LUMO: 0.80001 factor:1 | 1 (-1.57195) | -1 | -1 |
| G: -2104.18652 HOMO: -7.74164 LUMO: 1.37690 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10474.71439 HOMO: -6.52257 LUMO: 0.99049 factor:1 | 1 (-1.97566) | -1 | -1 |
| G: -2104.18652 HOMO: -7.74164 LUMO: 1.37690 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10474.82286 HOMO: -6.84638 LUMO: 1.10750 factor:1 | 1 (-2.08412) | -1 | -1 |
| G: -2104.18652 HOMO: -7.74164 LUMO: 1.37690 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10474.44350 HOMO: -6.85455 LUMO: 0.84900 factor:1 | 1 (-1.70477) | -1 | -1 |
| G: -2104.18652 HOMO: -7.74164 LUMO: 1.37690 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10475.40698 HOMO: -6.60148 LUMO: -0.78369 factor:1 | 1 (-2.66824) | -1 | -1 |
| G: -2104.18652 HOMO: -7.74164 LUMO: 1.37690 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10475.62464 HOMO: -6.86543 LUMO: -0.93063 factor:1 | 1 (-2.88590) | -1 | -1 |
| G: -2104.18652 HOMO: -7.74164 LUMO: 1.37690 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10475.72094 HOMO: -6.70489 LUMO: -0.72382 factor:1 | 1 (-2.98220) | -1 | -1 |
| G: -2104.18652 HOMO: -7.74164 LUMO: 1.37690 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10475.77822 HOMO: -6.59060 LUMO: 0.31293 factor:1 | 1 (-3.03948) | -1 | -1 |
| G: -2104.18652 HOMO: -7.74164 LUMO: 1.37690 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10475.61762 HOMO: -6.52257 LUMO: -0.48708 factor:1 | 1 (-2.87888) | -1 | -1 |
| G: -2104.18652 HOMO: -7.74164 LUMO: 1.37690 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10475.65795 HOMO: -6.54706 LUMO: -0.48164 factor:1 | 1 (-2.91921) | -1 | -1 |
| G: -2104.18652 HOMO: -7.74164 LUMO: 1.37690 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10476.06761 HOMO: -7.32803 LUMO: 0.08436 factor:1 | 1 (-3.32888) | -1 | -1 |
| G: -2104.18652 HOMO: -7.74164 LUMO: 1.37690 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10475.70584 HOMO: -6.77291 LUMO: -0.66940 factor:1 | 1 (-2.96710) | -1 | -1 |
| G: -2104.18652 HOMO: -7.74164 LUMO: 1.37690 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10475.54151 HOMO: -6.68312 LUMO: -0.53062 factor:1 | 1 (-2.80277) | -1 | -1 |
| G: -2104.18652 HOMO: -7.74164 LUMO: 1.37690 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10477.24502 HOMO: -7.07768 LUMO: 0.45987 factor:1 | 1 (-4.50629) | -1 | -1 |
| G: -2104.18652 HOMO: -7.74164 LUMO: 1.37690 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10476.41230 HOMO: -6.50352 LUMO: -0.63675 factor:1 | 1 (-3.67356) | -1 | -1 |
| G: -2104.18652 HOMO: -7.74164 LUMO: 1.37690 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10476.60735 HOMO: -6.48992 LUMO: -0.60681 factor:1 | 1 (-3.86862) | -1 | -1 |
| G: -2104.18652 HOMO: -7.74164 LUMO: 1.37690 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10476.74183 HOMO: -6.65318 LUMO: -0.72382 factor:1 | 1 (-4.00309) | -1 | -1 |
| G: -2104.18652 HOMO: -7.74164 LUMO: 1.37690 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10475.85515 HOMO: -6.54706 LUMO: 0.24218 factor:1 | 1 (-3.11641) | -1 | -1 |
| G: -2104.18652 HOMO: -7.74164 LUMO: 1.37690 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10475.81381 HOMO: -6.63958 LUMO: 0.57416 factor:1 | 1 (-3.07508) | -1 | -1 |
| G: -2104.18652 HOMO: -7.74164 LUMO: 1.37690 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10475.98544 HOMO: -6.37563 LUMO: -0.48164 factor:1 | 1 (-3.24670) | -1 | -1 |
| G: -2104.18652 HOMO: -7.74164 LUMO: 1.37690 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10476.03501 HOMO: -6.64774 LUMO: -0.71838 factor:1 | 1 (-3.29628) | -1 | -1 |
| G: -2104.18652 HOMO: -7.74164 LUMO: 1.37690 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10476.86123 HOMO: -7.17020 LUMO: 0.45987 factor:1 | 1 (-4.12250) | -1 | -1 |
| G: -2104.18652 HOMO: -7.74164 LUMO: 1.37690 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10476.34457 HOMO: -6.86543 LUMO: -1.05036 factor:1 | 1 (-3.60584) | -1 | -1 |
| G: -2104.18652 HOMO: -7.74164 LUMO: 1.37690 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10476.70202 HOMO: -6.77019 LUMO: -1.03131 factor:1 | 1 (-3.96328) | -1 | -1 |
| G: -2104.18652 HOMO: -7.74164 LUMO: 1.37690 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10474.83333 HOMO: -6.80285 LUMO: 1.05852 factor:1 | 1 (-2.09460) | -1 | -1 |
| G: -2104.18652 HOMO: -7.74164 LUMO: 1.37690 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10474.60097 HOMO: -6.76475 LUMO: 1.01771 factor:1 | 1 (-1.86224) | -1 | -1 |
| G: -2104.18652 HOMO: -7.74164 LUMO: 1.37690 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10474.32358 HOMO: -6.92530 LUMO: 1.37417 factor:1 | 1 (-1.58485) | -1 | -1 |
| G: -2104.18652 HOMO: -7.74164 LUMO: 1.37690 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10474.52576 HOMO: -6.98244 LUMO: 1.25989 factor:1 | 1 (-1.78703) | -1 | -1 |
| G: -2104.18652 HOMO: -7.74164 LUMO: 1.37690 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10475.02501 HOMO: -6.74842 LUMO: 0.89798 factor:1 | 1 (-2.28627) | -1 | -1 |
| G: -2104.18652 HOMO: -7.74164 LUMO: 1.37690 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10476.67277 HOMO: -6.77019 LUMO: -1.17009 factor:1 | 1 (-3.93403) | -1 | -1 |
| G: -2104.18652 HOMO: -7.74164 LUMO: 1.37690 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10474.69091 HOMO: -6.78652 LUMO: 1.35785 factor:1 | 1 (-1.95217) | -1 | -1 |
| G: -2104.18652 HOMO: -7.74164 LUMO: 1.37690 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10476.68531 HOMO: -6.82734 LUMO: -0.68301 factor:1 | 1 (-3.94658) | -1 | -1 |
| G: -2104.18652 HOMO: -7.74164 LUMO: 1.37690 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10476.93922 HOMO: -6.48175 LUMO: -2.19052 factor:1 | 1 (-4.20049) | -1 | -1 |
| G: -2104.18652 HOMO: -7.74164 LUMO: 1.37690 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10477.00363 HOMO: -6.65863 LUMO: -0.77008 factor:1 | 1 (-4.26489) | -1 | -1 |
| G: -2104.18652 HOMO: -7.74164 LUMO: 1.37690 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10476.90899 HOMO: -6.44094 LUMO: -2.20956 factor:1 | 1 (-4.17025) | -1 | -1 |
| G: -2104.18652 HOMO: -7.74164 LUMO: 1.37690 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10475.58630 HOMO: -6.59876 LUMO: -0.57688 factor:1 | 1 (-2.84756) | -1 | -1 |
| G: -2104.18652 HOMO: -7.74164 LUMO: 1.37690 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10475.31927 HOMO: -6.78380 LUMO: -0.77008 factor:1 | 1 (-2.58054) | -1 | -1 |
| G: -2104.18652 HOMO: -7.74164 LUMO: 1.37690 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10476.17167 HOMO: -7.30354 LUMO: 0.25034 factor:1 | 1 (-3.43293) | -1 | -1 |
| G: -2104.18652 HOMO: -7.74164 LUMO: 1.37690 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10475.62965 HOMO: -6.59332 LUMO: -0.53334 factor:1 | 1 (-2.89091) | -1 | -1 |
| G: -2104.18652 HOMO: -7.74164 LUMO: 1.37690 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10475.46679 HOMO: -6.64230 LUMO: -0.55783 factor:1 | 1 (-2.72805) | -1 | -1 |
| G: -2104.18652 HOMO: -7.74164 LUMO: 1.37690 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10476.10217 HOMO: -7.26544 LUMO: 0.20409 factor:1 | 1 (-3.36344) | -1 | -1 |
| G: -2104.18652 HOMO: -7.74164 LUMO: 1.37690 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10475.54186 HOMO: -6.61237 LUMO: -0.65307 factor:1 | 1 (-2.80313) | -1 | -1 |
| G: -2104.18652 HOMO: -7.74164 LUMO: 1.37690 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10475.69667 HOMO: -6.72393 LUMO: -0.65307 factor:1 | 1 (-2.95793) | -1 | -1 |
| G: -2104.18652 HOMO: -7.74164 LUMO: 1.37690 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10475.92181 HOMO: -6.29671 LUMO: -0.39729 factor:1 | 1 (-3.18308) | -1 | -1 |
| G: -2104.18652 HOMO: -7.74164 LUMO: 1.37690 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10475.65305 HOMO: -6.75387 LUMO: -0.53334 factor:1 | 1 (-2.91431) | -1 | -1 |
| G: -2104.18652 HOMO: -7.74164 LUMO: 1.37690 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10475.95735 HOMO: -6.53073 LUMO: -0.31293 factor:1 | 1 (-3.21862) | -1 | -1 |
| G: -2104.18652 HOMO: -7.74164 LUMO: 1.37690 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10476.02057 HOMO: -6.42189 LUMO: -0.59049 factor:1 | 1 (-3.28183) | -1 | -1 |
| G: -2104.18652 HOMO: -7.74164 LUMO: 1.37690 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10476.02979 HOMO: -6.41100 LUMO: -0.29933 factor:1 | 1 (-3.29105) | -1 | -1 |
| G: -2104.18652 HOMO: -7.74164 LUMO: 1.37690 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10476.04829 HOMO: -6.57427 LUMO: -0.53879 factor:1 | 1 (-3.30956) | -1 | -1 |
| G: -2104.18652 HOMO: -7.74164 LUMO: 1.37690 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10476.74001 HOMO: -7.43143 LUMO: 0.33470 factor:1 | 1 (-4.00127) | -1 | -1 |
| G: -2104.18652 HOMO: -7.74164 LUMO: 1.37690 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10475.95580 HOMO: -6.56067 LUMO: -0.50885 factor:1 | 1 (-3.21707) | -1 | -1 |
| G: -2104.18652 HOMO: -7.74164 LUMO: 1.37690 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10475.98261 HOMO: -6.65863 LUMO: -0.76464 factor:1 | 1 (-3.24387) | -1 | -1 |
| G: -2104.18652 HOMO: -7.74164 LUMO: 1.37690 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10475.95011 HOMO: -6.32665 LUMO: -0.41906 factor:1 | 1 (-3.21138) | -1 | -1 |
| G: -2104.18652 HOMO: -7.74164 LUMO: 1.37690 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10473.55206 HOMO: -6.57699 LUMO: 1.63813 factor:1 | 1 (-0.81332) | -1 | -1 |
| G: -2104.18652 HOMO: -7.74164 LUMO: 1.37690 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10474.16355 HOMO: -6.53073 LUMO: 1.71704 factor:1 | 1 (-1.42482) | -1 | -1 |
| G: -2104.18652 HOMO: -7.74164 LUMO: 1.37690 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10473.86278 HOMO: -6.86271 LUMO: 2.07351 factor:1 | 1 (-1.12405) | -1 | -1 |
| G: -2104.18652 HOMO: -7.74164 LUMO: 1.37690 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10474.70323 HOMO: -6.63686 LUMO: 1.78235 factor:1 | 1 (-1.96450) | -1 | -1 |
| G: -2104.18652 HOMO: -7.74164 LUMO: 1.37690 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10474.65638 HOMO: -6.60965 LUMO: 1.94289 factor:1 | 1 (-1.91764) | -1 | -1 |
| G: -2104.18652 HOMO: -7.74164 LUMO: 1.37690 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10474.61398 HOMO: -6.55250 LUMO: 1.89119 factor:1 | 1 (-1.87525) | -1 | -1 |
| G: -2104.18652 HOMO: -7.74164 LUMO: 1.37690 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10474.56933 HOMO: -6.50624 LUMO: 1.85582 factor:1 | 1 (-1.83059) | -1 | -1 |
| G: -2104.18652 HOMO: -7.74164 LUMO: 1.37690 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10474.45765 HOMO: -6.06814 LUMO: 1.94561 factor:1 | 1 (-1.71892) | -1 | -1 |
| G: -2104.18652 HOMO: -7.74164 LUMO: 1.37690 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10475.07043 HOMO: -6.58788 LUMO: 2.01908 factor:1 | 1 (-2.33169) | -1 | -1 |
| G: -2104.18652 HOMO: -7.74164 LUMO: 1.37690 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10475.88530 HOMO: -6.74026 LUMO: 0.31293 factor:1 | 1 (-3.14656) | -1 | -1 |
| G: -2104.18652 HOMO: -7.74164 LUMO: 1.37690 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10476.58305 HOMO: -6.54434 LUMO: -0.42994 factor:1 | 1 (-3.84432) | -1 | -1 |
| G: -2104.18652 HOMO: -7.74164 LUMO: 1.37690 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10477.21817 HOMO: -6.94707 LUMO: 0.42994 factor:1 | 1 (-4.47943) | -1 | -1 |
| G: -2104.18652 HOMO: -7.74164 LUMO: 1.37690 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10477.10469 HOMO: -6.98516 LUMO: 0.41361 factor:1 | 1 (-4.36596) | -1 | -1 |
| G: -2104.18652 HOMO: -7.74164 LUMO: 1.37690 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10476.36569 HOMO: -6.31304 LUMO: -0.54967 factor:1 | 1 (-3.62695) | -1 | -1 |
| G: -2104.18652 HOMO: -7.74164 LUMO: 1.37690 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10476.68844 HOMO: -6.48447 LUMO: -0.40817 factor:1 | 1 (-3.94971) | -1 | -1 |
| G: -2104.18652 HOMO: -7.74164 LUMO: 1.37690 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10475.76551 HOMO: -6.49264 LUMO: 0.29116 factor:1 | 1 (-3.02678) | -1 | -1 |
| G: -2104.18652 HOMO: -7.74164 LUMO: 1.37690 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10475.78271 HOMO: -6.48719 LUMO: -0.11973 factor:1 | 1 (-3.04397) | -1 | -1 |
| G: -2104.18652 HOMO: -7.74164 LUMO: 1.37690 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10476.45774 HOMO: -7.16204 LUMO: 0.44082 factor:1 | 1 (-3.71901) | -1 | -1 |
| G: -2104.18652 HOMO: -7.74164 LUMO: 1.37690 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10475.87085 HOMO: -6.74842 LUMO: -0.37552 factor:1 | 1 (-3.13211) | -1 | -1 |
| G: -2104.18652 HOMO: -7.74164 LUMO: 1.37690 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10476.58996 HOMO: -6.44638 LUMO: -0.45171 factor:1 | 1 (-3.85123) | -1 | -1 |
| G: -2104.18652 HOMO: -7.74164 LUMO: 1.37690 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10477.31594 HOMO: -7.07496 LUMO: 0.50341 factor:1 | 1 (-4.57720) | -1 | -1 |
| G: -2104.18652 HOMO: -7.74164 LUMO: 1.37690 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10476.06331 HOMO: -6.79468 LUMO: 0.11429 factor:1 | 1 (-3.32458) | -1 | -1 |
| G: -2104.18652 HOMO: -7.74164 LUMO: 1.37690 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10476.58773 HOMO: -6.63958 LUMO: -0.67484 factor:1 | 1 (-3.84900) | -1 | -1 |
| G: -2104.18652 HOMO: -7.74164 LUMO: 1.37690 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10477.42742 HOMO: -7.08584 LUMO: 0.46259 factor:1 | 1 (-4.68869) | -1 | -1 |
| G: -2104.18652 HOMO: -7.74164 LUMO: 1.37690 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10476.67533 HOMO: -6.80285 LUMO: -0.73199 factor:1 | 1 (-3.93659) | -1 | -1 |
| G: -2104.18652 HOMO: -7.74164 LUMO: 1.37690 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10476.66104 HOMO: -6.44366 LUMO: -0.45443 factor:1 | 1 (-3.92230) | -1 | -1 |
| G: -2104.18652 HOMO: -7.74164 LUMO: 1.37690 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10475.99373 HOMO: -6.75931 LUMO: 0.25851 factor:1 | 1 (-3.25500) | -1 | -1 |
| G: -2104.18652 HOMO: -7.74164 LUMO: 1.37690 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10474.76854 HOMO: -6.64502 LUMO: 1.79323 factor:1 | 1 (-2.02981) | -1 | -1 |
| G: -2104.18652 HOMO: -7.74164 LUMO: 1.37690 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10474.53918 HOMO: -6.51168 LUMO: 1.60275 factor:1 | 1 (-1.80044) | -1 | -1 |
| G: -2104.18652 HOMO: -7.74164 LUMO: 1.37690 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10474.68859 HOMO: -6.56067 LUMO: 1.63268 factor:1 | 1 (-1.94986) | -1 | -1 |
| G: -2104.18652 HOMO: -7.74164 LUMO: 1.37690 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10474.78928 HOMO: -6.56883 LUMO: 1.70615 factor:1 | 1 (-2.05054) | -1 | -1 |
| G: -2104.18652 HOMO: -7.74164 LUMO: 1.37690 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10474.74457 HOMO: -6.77836 LUMO: 1.77962 factor:1 | 1 (-2.00583) | -1 | -1 |
| G: -2104.18652 HOMO: -7.74164 LUMO: 1.37690 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10473.74033 HOMO: -6.38923 LUMO: 1.85854 factor:1 | 1 (-1.00160) | -1 | -1 |
| G: -2104.18652 HOMO: -7.74164 LUMO: 1.37690 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10473.64841 HOMO: -6.35658 LUMO: 2.16875 factor:1 | 1 (-0.90968) | -1 | -1 |
| G: -2104.18652 HOMO: -7.74164 LUMO: 1.37690 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10473.98404 HOMO: -6.83006 LUMO: 2.31025 factor:1 | 1 (-1.24530) | -1 | -1 |
| G: -2104.18652 HOMO: -7.74164 LUMO: 1.37690 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10474.03321 HOMO: -6.87087 LUMO: 1.79051 factor:1 | 1 (-1.29447) | -1 | -1 |
| G: -2104.18652 HOMO: -7.74164 LUMO: 1.37690 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10475.13943 HOMO: -6.56339 LUMO: 2.37828 factor:1 | 1 (-2.40070) | -1 | -1 |
| G: -2104.18652 HOMO: -7.74164 LUMO: 1.37690 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10475.26425 HOMO: -6.30488 LUMO: 2.51705 factor:1 | 1 (-2.52552) | -1 | -1 |
| G: -2104.18652 HOMO: -7.74164 LUMO: 1.37690 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10475.22817 HOMO: -6.69400 LUMO: 1.95650 factor:1 | 1 (-2.48943) | -1 | -1 |
| G: -2104.18652 HOMO: -7.74164 LUMO: 1.37690 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10475.21949 HOMO: -6.51168 LUMO: 2.03541 factor:1 | 1 (-2.48075) | -1 | -1 |
| G: -2104.18652 HOMO: -7.74164 LUMO: 1.37690 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10474.78803 HOMO: -6.30760 LUMO: 1.65173 factor:1 | 1 (-2.04929) | -1 | -1 |
| G: -2104.18652 HOMO: -7.74164 LUMO: 1.37690 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10474.60952 HOMO: -6.55250 LUMO: 1.90752 factor:1 | 1 (-1.87078) | -1 | -1 |
| G: -2104.18652 HOMO: -7.74164 LUMO: 1.37690 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10474.57341 HOMO: -6.41372 LUMO: 1.76058 factor:1 | 1 (-1.83467) | -1 | -1 |
| G: -2104.18652 HOMO: -7.74164 LUMO: 1.37690 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10474.62465 HOMO: -6.23957 LUMO: 2.06534 factor:1 | 1 (-1.88591) | -1 | -1 |
| G: -2104.18652 HOMO: -7.74164 LUMO: 1.37690 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10475.59770 HOMO: -6.58243 LUMO: 2.11705 factor:1 | 1 (-2.85896) | -1 | -1 |
| G: -2104.18652 HOMO: -7.74164 LUMO: 1.37690 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10475.26945 HOMO: -6.37835 LUMO: 2.09256 factor:1 | 1 (-2.53071) | -1 | -1 |
| G: -2104.18652 HOMO: -7.74164 LUMO: 1.37690 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10475.41732 HOMO: -6.50624 LUMO: 2.55787 factor:1 | 1 (-2.67858) | -1 | -1 |
| G: -2104.18652 HOMO: -7.74164 LUMO: 1.37690 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10475.44387 HOMO: -6.45454 LUMO: 1.87214 factor:1 | 1 (-2.70514) | -1 | -1 |
| G: -2104.18652 HOMO: -7.74164 LUMO: 1.37690 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10475.19315 HOMO: -6.53617 LUMO: 1.95650 factor:1 | 1 (-2.45441) | -1 | -1 |
| G: -2104.18652 HOMO: -7.74164 LUMO: 1.37690 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10475.06906 HOMO: -6.51985 LUMO: 1.71432 factor:1 | 1 (-2.33033) | -1 | -1 |
| G: -2104.18652 HOMO: -7.74164 LUMO: 1.37690 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10475.31201 HOMO: -6.75114 LUMO: 1.84493 factor:1 | 1 (-2.57327) | -1 | -1 |
| G: -2104.18652 HOMO: -7.74164 LUMO: 1.37690 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10474.33926 HOMO: -6.06270 LUMO: 1.65717 factor:1 | 1 (-1.60052) | -1 | -1 |
| G: -2104.18652 HOMO: -7.74164 LUMO: 1.37690 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10474.70734 HOMO: -5.89671 LUMO: 1.71704 factor:1 | 1 (-1.96861) | -1 | -1 |
| G: -2104.18652 HOMO: -7.74164 LUMO: 1.37690 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10474.52160 HOMO: -6.18787 LUMO: 1.91840 factor:1 | 1 (-1.78286) | -1 | -1 |
| G: -2104.18652 HOMO: -7.74164 LUMO: 1.37690 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10474.39281 HOMO: -6.01644 LUMO: 1.85582 factor:1 | 1 (-1.65407) | -1 | -1 |
| G: -2104.18652 HOMO: -7.74164 LUMO: 1.37690 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10475.32107 HOMO: -6.05998 LUMO: 2.33474 factor:1 | 1 (-2.58233) | -1 | -1 |
| G: -2104.18652 HOMO: -7.74164 LUMO: 1.37690 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10475.35568 HOMO: -6.05725 LUMO: 2.03541 factor:1 | 1 (-2.61695) | -1 | -1 |
| G: -2104.18652 HOMO: -7.74164 LUMO: 1.37690 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10475.37451 HOMO: -6.80829 LUMO: 1.90480 factor:1 | 1 (-2.63578) | -1 | -1 |
| G: -2104.18652 HOMO: -7.74164 LUMO: 1.37690 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10475.59250 HOMO: -6.76475 LUMO: 2.20956 factor:1 | 1 (-2.85377) | -1 | -1 |
| G: -2104.18652 HOMO: -7.74164 LUMO: 1.37690 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10475.51457 HOMO: -6.29944 LUMO: 1.77962 factor:1 | 1 (-2.77583) | -1 | -1 |
| G: -2104.18652 HOMO: -7.74164 LUMO: 1.37690 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10475.78097 HOMO: -6.47359 LUMO: -0.25579 factor:1 | 1 (-3.04223) | -1 | -1 |
| G: -2104.18652 HOMO: -7.74164 LUMO: 1.37690 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10475.69667 HOMO: -6.57699 LUMO: -0.47348 factor:1 | 1 (-2.95793) | -1 | -1 |
| G: -2104.18652 HOMO: -7.74164 LUMO: 1.37690 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10476.60058 HOMO: -7.20830 LUMO: 0.49797 factor:1 | 1 (-3.86184) | -1 | -1 |
| G: -2104.18652 HOMO: -7.74164 LUMO: 1.37690 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10476.16021 HOMO: -7.49402 LUMO: 0.29933 factor:1 | 1 (-3.42148) | -1 | -1 |
| G: -2104.18652 HOMO: -7.74164 LUMO: 1.37690 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10475.65117 HOMO: -6.66679 LUMO: -0.58777 factor:1 | 1 (-2.91243) | -1 | -1 |
| G: -2104.18652 HOMO: -7.74164 LUMO: 1.37690 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10475.54398 HOMO: -6.67767 LUMO: -0.56328 factor:1 | 1 (-2.80525) | -1 | -1 |
| G: -2104.18652 HOMO: -7.74164 LUMO: 1.37690 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10476.77027 HOMO: -7.42871 LUMO: 0.35647 factor:1 | 1 (-4.03153) | -1 | -1 |
| G: -2104.18652 HOMO: -7.74164 LUMO: 1.37690 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10475.78442 HOMO: -6.56067 LUMO: -0.54423 factor:1 | 1 (-3.04569) | -1 | -1 |
| G: -2104.18652 HOMO: -7.74164 LUMO: 1.37690 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10475.61514 HOMO: -6.56339 LUMO: -0.50341 factor:1 | 1 (-2.87641) | -1 | -1 |
| G: -2104.18652 HOMO: -7.74164 LUMO: 1.37690 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10475.77833 HOMO: -6.56067 LUMO: -0.48436 factor:1 | 1 (-3.03959) | -1 | -1 |
| G: -2104.18652 HOMO: -7.74164 LUMO: 1.37690 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10474.72500 HOMO: -6.73210 LUMO: 1.75241 factor:1 | 1 (-1.98627) | -1 | -1 |
| G: -2104.18652 HOMO: -7.74164 LUMO: 1.37690 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10474.79156 HOMO: -6.48175 LUMO: 1.91296 factor:1 | 1 (-2.05283) | -1 | -1 |
| G: -2104.18652 HOMO: -7.74164 LUMO: 1.37690 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10474.54576 HOMO: -6.67767 LUMO: 1.70343 factor:1 | 1 (-1.80703) | -1 | -1 |
| G: -2104.18652 HOMO: -7.74164 LUMO: 1.37690 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10473.36683 HOMO: -6.37835 LUMO: 1.96466 factor:1 | 1 (-0.62809) | -1 | -1 |
| G: -2104.18652 HOMO: -7.74164 LUMO: 1.37690 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10473.65769 HOMO: -6.40828 LUMO: 2.10072 factor:1 | 1 (-0.91896) | -1 | -1 |
| G: -2104.18652 HOMO: -7.74164 LUMO: 1.37690 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10474.66389 HOMO: -6.06542 LUMO: 1.92112 factor:1 | 1 (-1.92515) | -1 | -1 |
| G: -2104.18652 HOMO: -7.74164 LUMO: 1.37690 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10474.84618 HOMO: -6.90353 LUMO: 1.83133 factor:1 | 1 (-2.10744) | -1 | -1 |
| G: -2104.18652 HOMO: -7.74164 LUMO: 1.37690 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10474.57322 HOMO: -6.37019 LUMO: 1.92929 factor:1 | 1 (-1.83448) | -1 | -1 |
| G: -2104.18652 HOMO: -7.74164 LUMO: 1.37690 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10473.81209 HOMO: -6.61509 LUMO: 2.11160 factor:1 | 1 (-1.07335) | -1 | -1 |
| G: -2104.18652 HOMO: -7.74164 LUMO: 1.37690 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10474.75145 HOMO: -6.82734 LUMO: 1.77146 factor:1 | 1 (-2.01272) | -1 | -1 |
| G: -2104.18652 HOMO: -7.74164 LUMO: 1.37690 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10474.51673 HOMO: -6.01100 LUMO: 1.89935 factor:1 | 1 (-1.77799) | -1 | -1 |
| G: -2104.18652 HOMO: -7.74164 LUMO: 1.37690 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10474.49738 HOMO: -6.49536 LUMO: 1.75241 factor:1 | 1 (-1.75864) | -1 | -1 |
| G: -2104.18652 HOMO: -7.74164 LUMO: 1.37690 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10474.50753 HOMO: -6.34297 LUMO: 1.86398 factor:1 | 1 (-1.76879) | -1 | -1 |
| G: -2104.18652 HOMO: -7.74164 LUMO: 1.37690 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10474.62242 HOMO: -6.53073 LUMO: 1.84493 factor:1 | 1 (-1.88368) | -1 | -1 |
| G: -2104.18652 HOMO: -7.74164 LUMO: 1.37690 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10475.36997 HOMO: -6.53345 LUMO: 2.41093 factor:1 | 1 (-2.63123) | -1 | -1 |
| G: -2104.18652 HOMO: -7.74164 LUMO: 1.37690 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10475.55639 HOMO: -7.01237 LUMO: 2.06262 factor:1 | 1 (-2.81766) | -1 | -1 |
| G: -2104.18652 HOMO: -7.74164 LUMO: 1.37690 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10474.55828 HOMO: -6.17154 LUMO: 1.89119 factor:1 | 1 (-1.81954) | -1 | -1 |
| G: -2104.18652 HOMO: -7.74164 LUMO: 1.37690 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10474.82966 HOMO: -6.08719 LUMO: 1.74425 factor:1 | 1 (-2.09092) | -1 | -1 |
| G: -2104.18652 HOMO: -7.74164 LUMO: 1.37690 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10474.86419 HOMO: -6.69672 LUMO: 1.95106 factor:1 | 1 (-2.12545) | -1 | -1 |
| G: -2104.18652 HOMO: -7.74164 LUMO: 1.37690 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10475.27037 HOMO: -6.58243 LUMO: 2.24766 factor:1 | 1 (-2.53164) | -1 | -1 |
| G: -2104.18652 HOMO: -7.74164 LUMO: 1.37690 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10475.24632 HOMO: -6.74570 LUMO: 2.02181 factor:1 | 1 (-2.50758) | -1 | -1 |
| G: -2104.18652 HOMO: -7.74164 LUMO: 1.37690 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10474.94781 HOMO: -6.53890 LUMO: 1.92929 factor:1 | 1 (-2.20907) | -1 | -1 |
| G: -2104.18652 HOMO: -7.74164 LUMO: 1.37690 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10474.79676 HOMO: -6.03276 LUMO: 1.67078 factor:1 | 1 (-2.05802) | -1 | -1 |
| G: -2104.18652 HOMO: -7.74164 LUMO: 1.37690 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10474.77322 HOMO: -6.67767 LUMO: 2.03541 factor:1 | 1 (-2.03449) | -1 | -1 |
| G: -2104.18652 HOMO: -7.74164 LUMO: 1.37690 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10474.65956 HOMO: -5.98378 LUMO: 1.84221 factor:1 | 1 (-1.92082) | -1 | -1 |
| G: -2104.18652 HOMO: -7.74164 LUMO: 1.37690 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10474.67327 HOMO: -6.07086 LUMO: 2.01908 factor:1 | 1 (-1.93454) | -1 | -1 |
| G: -2104.18652 HOMO: -7.74164 LUMO: 1.37690 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10474.04581 HOMO: -6.29944 LUMO: 1.90208 factor:1 | 1 (-1.30707) | -1 | -1 |
| G: -2104.18652 HOMO: -7.74164 LUMO: 1.37690 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10474.26306 HOMO: -6.75114 LUMO: 1.85854 factor:1 | 1 (-1.52433) | -1 | -1 |
| G: -2104.18652 HOMO: -7.74164 LUMO: 1.37690 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10475.17375 HOMO: -6.56611 LUMO: 2.49801 factor:1 | 1 (-2.43501) | -1 | -1 |
| G: -2104.18652 HOMO: -7.74164 LUMO: 1.37690 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10475.29837 HOMO: -6.39740 LUMO: 1.92929 factor:1 | 1 (-2.55964) | -1 | -1 |
| G: -2104.18652 HOMO: -7.74164 LUMO: 1.37690 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10476.28996 HOMO: -6.85999 LUMO: -1.07757 factor:1 | 1 (-3.55122) | -1 | -1 |
| G: -2104.18652 HOMO: -7.74164 LUMO: 1.37690 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10474.57374 HOMO: -6.98244 LUMO: 1.07213 factor:1 | 1 (-1.83500) | -1 | -1 |
| G: -2104.18652 HOMO: -7.74164 LUMO: 1.37690 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10474.67673 HOMO: -7.04231 LUMO: 0.64219 factor:1 | 1 (-1.93799) | -1 | -1 |
| G: -2104.18652 HOMO: -7.74164 LUMO: 1.37690 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10474.33836 HOMO: -6.96339 LUMO: 0.75648 factor:1 | 1 (-1.59962) | -1 | -1 |
| G: -2104.18652 HOMO: -7.74164 LUMO: 1.37690 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10476.31899 HOMO: -6.83822 LUMO: -0.97417 factor:1 | 1 (-3.58026) | -1 | -1 |
| G: -2104.18652 HOMO: -7.74164 LUMO: 1.37690 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10476.96104 HOMO: -6.44910 LUMO: -2.15242 factor:1 | 1 (-4.22231) | -1 | -1 |
| G: -2104.18652 HOMO: -7.74164 LUMO: 1.37690 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10476.75639 HOMO: -6.84094 LUMO: -1.37690 factor:1 | 1 (-4.01765) | -1 | -1 |
| G: -2104.18652 HOMO: -7.74164 LUMO: 1.37690 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10476.46765 HOMO: -6.74026 LUMO: -2.54699 factor:1 | 1 (-3.72891) | -1 | -1 |
| G: -2104.18652 HOMO: -7.74164 LUMO: 1.37690 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10474.53344 HOMO: -6.96611 LUMO: 1.24900 factor:1 | 1 (-1.79470) | -1 | -1 |
| G: -2104.18652 HOMO: -7.74164 LUMO: 1.37690 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10474.47752 HOMO: -7.21102 LUMO: 0.82995 factor:1 | 1 (-1.73878) | -1 | -1 |
| G: -2104.18652 HOMO: -7.74164 LUMO: 1.37690 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10474.57978 HOMO: -6.88448 LUMO: 0.81634 factor:1 | 1 (-1.84104) | -1 | -1 |
| G: -2104.18652 HOMO: -7.74164 LUMO: 1.37690 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10474.36451 HOMO: -7.04231 LUMO: 1.10750 factor:1 | 1 (-1.62577) | -1 | -1 |
| G: -2104.18652 HOMO: -7.74164 LUMO: 1.37690 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10476.33793 HOMO: -6.83550 LUMO: -0.98777 factor:1 | 1 (-3.59920) | -1 | -1 |
| G: -2104.18652 HOMO: -7.74164 LUMO: 1.37690 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10474.70051 HOMO: -6.82189 LUMO: 0.93879 factor:1 | 1 (-1.96178) | -1 | -1 |
| G: -2104.18652 HOMO: -7.74164 LUMO: 1.37690 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10474.92414 HOMO: -6.81101 LUMO: 0.70750 factor:1 | 1 (-2.18540) | -1 | -1 |
| G: -2104.18652 HOMO: -7.74164 LUMO: 1.37690 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10474.73692 HOMO: -7.06680 LUMO: 0.74015 factor:1 | 1 (-1.99819) | -1 | -1 |
| G: -2104.18652 HOMO: -7.74164 LUMO: 1.37690 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10474.30671 HOMO: -6.68856 LUMO: 0.86260 factor:1 | 1 (-1.56797) | -1 | -1 |
| G: -2104.18652 HOMO: -7.74164 LUMO: 1.37690 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10476.75976 HOMO: -6.83822 LUMO: -0.63403 factor:1 | 1 (-4.02103) | -1 | -1 |
| G: -2104.18652 HOMO: -7.74164 LUMO: 1.37690 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10475.03483 HOMO: -6.84911 LUMO: 1.26533 factor:1 | 1 (-2.29610) | -1 | -1 |
| G: -2104.18652 HOMO: -7.74164 LUMO: 1.37690 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10474.33291 HOMO: -7.01237 LUMO: 0.73743 factor:1 | 1 (-1.59418) | -1 | -1 |
| G: -2104.18652 HOMO: -7.74164 LUMO: 1.37690 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10474.64351 HOMO: -7.00965 LUMO: 1.40139 factor:1 | 1 (-1.90477) | -1 | -1 |
| G: -2104.18652 HOMO: -7.74164 LUMO: 1.37690 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10476.33488 HOMO: -6.73210 LUMO: -2.49256 factor:1 | 1 (-3.59615) | -1 | -1 |
| G: -2104.18652 HOMO: -7.74164 LUMO: 1.37690 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10474.33806 HOMO: -7.08040 LUMO: 0.84627 factor:1 | 1 (-1.59932) | -1 | -1 |
| G: -2104.18652 HOMO: -7.74164 LUMO: 1.37690 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10474.35792 HOMO: -7.00965 LUMO: 0.82995 factor:1 | 1 (-1.61919) | -1 | -1 |
| G: -2104.18652 HOMO: -7.74164 LUMO: 1.37690 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10474.25819 HOMO: -6.88448 LUMO: 0.82723 factor:1 | 1 (-1.51946) | -1 | -1 |
| G: -2104.18652 HOMO: -7.74164 LUMO: 1.37690 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10474.46119 HOMO: -7.20013 LUMO: 0.88437 factor:1 | 1 (-1.72245) | -1 | -1 |
| G: -2104.18652 HOMO: -7.74164 LUMO: 1.37690 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10475.66211 HOMO: -6.60420 LUMO: -0.53334 factor:1 | 1 (-2.92337) | -1 | -1 |
| G: -2104.18652 HOMO: -7.74164 LUMO: 1.37690 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10475.68665 HOMO: -6.78652 LUMO: -0.79729 factor:1 | 1 (-2.94792) | -1 | -1 |
| G: -2104.18652 HOMO: -7.74164 LUMO: 1.37690 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10475.50956 HOMO: -6.48992 LUMO: -0.64491 factor:1 | 1 (-2.77083) | -1 | -1 |
| G: -2104.18652 HOMO: -7.74164 LUMO: 1.37690 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10475.55098 HOMO: -6.85999 LUMO: -0.78097 factor:1 | 1 (-2.81224) | -1 | -1 |
| G: -2104.18652 HOMO: -7.74164 LUMO: 1.37690 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10475.93831 HOMO: -6.65046 LUMO: -0.78097 factor:1 | 1 (-3.19957) | -1 | -1 |
| G: -2104.18652 HOMO: -7.74164 LUMO: 1.37690 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10476.65413 HOMO: -7.24095 LUMO: 0.37280 factor:1 | 1 (-3.91539) | -1 | -1 |
| G: -2104.18652 HOMO: -7.74164 LUMO: 1.37690 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10475.88941 HOMO: -6.81101 LUMO: -0.74831 factor:1 | 1 (-3.15067) | -1 | -1 |
| G: -2104.18652 HOMO: -7.74164 LUMO: 1.37690 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10475.99341 HOMO: -6.69400 LUMO: -0.77280 factor:1 | 1 (-3.25467) | -1 | -1 |
| G: -2104.18652 HOMO: -7.74164 LUMO: 1.37690 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10475.64010 HOMO: -6.08447 LUMO: -0.68573 factor:1 | 1 (-2.90136) | -1 | -1 |
| G: -2104.18652 HOMO: -7.74164 LUMO: 1.37690 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10475.54309 HOMO: -6.66679 LUMO: -0.47076 factor:1 | 1 (-2.80435) | -1 | -1 |
| G: -2104.18652 HOMO: -7.74164 LUMO: 1.37690 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10475.59639 HOMO: -6.97428 LUMO: -1.10750 factor:1 | 1 (-2.85766) | -1 | -1 |
| G: -2104.18652 HOMO: -7.74164 LUMO: 1.37690 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10475.62450 HOMO: -6.69128 LUMO: -0.54151 factor:1 | 1 (-2.88577) | -1 | -1 |
| G: -2104.18652 HOMO: -7.74164 LUMO: 1.37690 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10475.39087 HOMO: -6.53617 LUMO: -0.35375 factor:1 | 1 (-2.65213) | -1 | -1 |
| G: -2104.18652 HOMO: -7.74164 LUMO: 1.37690 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10475.57517 HOMO: -6.75659 LUMO: -0.41361 factor:1 | 1 (-2.83643) | -1 | -1 |
| G: -2104.18652 HOMO: -7.74164 LUMO: 1.37690 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10475.69006 HOMO: -6.69400 LUMO: -0.67484 factor:1 | 1 (-2.95132) | -1 | -1 |
| G: -2104.18652 HOMO: -7.74164 LUMO: 1.37690 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10475.75417 HOMO: -6.89264 LUMO: -0.90886 factor:1 | 1 (-3.01543) | -1 | -1 |
| G: -2104.18652 HOMO: -7.74164 LUMO: 1.37690 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10475.43443 HOMO: -6.56339 LUMO: -0.52518 factor:1 | 1 (-2.69570) | -1 | -1 |
| G: -2104.18652 HOMO: -7.74164 LUMO: 1.37690 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10476.29067 HOMO: -6.45726 LUMO: -0.65852 factor:1 | 1 (-3.55193) | -1 | -1 |
| G: -2104.18652 HOMO: -7.74164 LUMO: 1.37690 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10476.12459 HOMO: -6.80557 LUMO: -0.56600 factor:1 | 1 (-3.38586) | -1 | -1 |
| G: -2104.18652 HOMO: -7.74164 LUMO: 1.37690 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10476.46958 HOMO: -7.19469 LUMO: -0.91702 factor:1 | 1 (-3.73084) | -1 | -1 |
| G: -2104.18652 HOMO: -7.74164 LUMO: 1.37690 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10475.81066 HOMO: -6.41100 LUMO: 0.79185 factor:1 | 1 (-3.07192) | -1 | -1 |
| G: -2104.18652 HOMO: -7.74164 LUMO: 1.37690 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10475.73128 HOMO: -6.39195 LUMO: 0.26123 factor:1 | 1 (-2.99254) | -1 | -1 |
| G: -2104.18652 HOMO: -7.74164 LUMO: 1.37690 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10475.67844 HOMO: -6.78924 LUMO: 0.35919 factor:1 | 1 (-2.93970) | -1 | -1 |
| G: -2104.18652 HOMO: -7.74164 LUMO: 1.37690 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10475.81166 HOMO: -6.50624 LUMO: 0.71838 factor:1 | 1 (-3.07293) | -1 | -1 |
| G: -2104.18652 HOMO: -7.74164 LUMO: 1.37690 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10475.47536 HOMO: -6.68584 LUMO: -0.66124 factor:1 | 1 (-2.73662) | -1 | -1 |
| G: -2104.18652 HOMO: -7.74164 LUMO: 1.37690 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10475.50115 HOMO: -6.45182 LUMO: -0.48980 factor:1 | 1 (-2.76242) | -1 | -1 |
| G: -2104.18652 HOMO: -7.74164 LUMO: 1.37690 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10475.60891 HOMO: -7.18925 LUMO: -1.01498 factor:1 | 1 (-2.87018) | -1 | -1 |
| G: -2104.18652 HOMO: -7.74164 LUMO: 1.37690 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10475.92976 HOMO: -7.18925 LUMO: -0.63130 factor:1 | 1 (-3.19102) | -1 | -1 |
| G: -2104.18652 HOMO: -7.74164 LUMO: 1.37690 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10475.88611 HOMO: -6.66679 LUMO: -0.57960 factor:1 | 1 (-3.14738) | -1 | -1 |
| G: -2104.18652 HOMO: -7.74164 LUMO: 1.37690 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10475.95101 HOMO: -6.44910 LUMO: -0.30205 factor:1 | 1 (-3.21228) | -1 | -1 |
| G: -2104.18652 HOMO: -7.74164 LUMO: 1.37690 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10476.48354 HOMO: -7.23279 LUMO: 0.46804 factor:1 | 1 (-3.74480) | -1 | -1 |
| G: -2104.18652 HOMO: -7.74164 LUMO: 1.37690 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10475.27856 HOMO: -6.92802 LUMO: -0.72927 factor:1 | 1 (-2.53983) | -1 | -1 |
| G: -2104.18652 HOMO: -7.74164 LUMO: 1.37690 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10475.53993 HOMO: -6.83278 LUMO: -0.59321 factor:1 | 1 (-2.80119) | -1 | -1 |
| G: -2104.18652 HOMO: -7.74164 LUMO: 1.37690 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10476.04141 HOMO: -7.44776 LUMO: 0.27211 factor:1 | 1 (-3.30267) | -1 | -1 |
| G: -2104.18652 HOMO: -7.74164 LUMO: 1.37690 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10475.49280 HOMO: -6.80829 LUMO: -0.59865 factor:1 | 1 (-2.75406) | -1 | -1 |
| G: -2104.18652 HOMO: -7.74164 LUMO: 1.37690 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10475.85517 HOMO: -6.63686 LUMO: -0.75103 factor:1 | 1 (-3.11644) | -1 | -1 |
| G: -2104.18652 HOMO: -7.74164 LUMO: 1.37690 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10475.70554 HOMO: -6.73210 LUMO: -0.55511 factor:1 | 1 (-2.96680) | -1 | -1 |
| G: -2104.18652 HOMO: -7.74164 LUMO: 1.37690 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10474.76519 HOMO: -6.50624 LUMO: 1.58642 factor:1 | 1 (-2.02646) | -1 | -1 |
| G: -2104.18652 HOMO: -7.74164 LUMO: 1.37690 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10474.68753 HOMO: -6.79196 LUMO: 0.96328 factor:1 | 1 (-1.94880) | -1 | -1 |
| G: -2104.18652 HOMO: -7.74164 LUMO: 1.37690 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10474.33920 HOMO: -6.82734 LUMO: 1.23540 factor:1 | 1 (-1.60046) | -1 | -1 |
| G: -2104.18652 HOMO: -7.74164 LUMO: 1.37690 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10474.53224 HOMO: -6.90081 LUMO: 1.25444 factor:1 | 1 (-1.79350) | -1 | -1 |
| G: -2104.18652 HOMO: -7.74164 LUMO: 1.37690 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10476.32288 HOMO: -7.00965 LUMO: -1.05036 factor:1 | 1 (-3.58415) | -1 | -1 |
| G: -2104.18652 HOMO: -7.74164 LUMO: 1.37690 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10476.35399 HOMO: -7.01237 LUMO: -1.48302 factor:1 | 1 (-3.61525) | -1 | -1 |
| G: -2104.18652 HOMO: -7.74164 LUMO: 1.37690 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10474.31003 HOMO: -6.91713 LUMO: 0.93607 factor:1 | 1 (-1.57129) | -1 | -1 |
| G: -2104.18652 HOMO: -7.74164 LUMO: 1.37690 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10474.21490 HOMO: -7.02598 LUMO: 0.92247 factor:1 | 1 (-1.47616) | -1 | -1 |
| G: -2104.18652 HOMO: -7.74164 LUMO: 1.37690 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10474.19106 HOMO: -6.98516 LUMO: 1.52384 factor:1 | 1 (-1.45233) | -1 | -1 |
| G: -2104.18652 HOMO: -7.74164 LUMO: 1.37690 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10473.91054 HOMO: -6.75387 LUMO: 1.04764 factor:1 | 1 (-1.17180) | -1 | -1 |
| G: -2104.18652 HOMO: -7.74164 LUMO: 1.37690 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10474.43259 HOMO: -7.09401 LUMO: 1.19458 factor:1 | 1 (-1.69385) | -1 | -1 |
| G: -2104.18652 HOMO: -7.74164 LUMO: 1.37690 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10476.27058 HOMO: -6.88992 LUMO: -1.56193 factor:1 | 1 (-3.53185) | -1 | -1 |
| G: -2104.18652 HOMO: -7.74164 LUMO: 1.37690 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10474.66397 HOMO: -7.00149 LUMO: 0.99866 factor:1 | 1 (-1.92523) | -1 | -1 |
| G: -2104.18652 HOMO: -7.74164 LUMO: 1.37690 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10474.30883 HOMO: -7.13755 LUMO: 1.05308 factor:1 | 1 (-1.57010) | -1 | -1 |
| G: -2104.18652 HOMO: -7.74164 LUMO: 1.37690 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10476.70460 HOMO: -6.85183 LUMO: -1.42860 factor:1 | 1 (-3.96587) | -1 | -1 |
| G: -2104.18652 HOMO: -7.74164 LUMO: 1.37690 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10475.54186 HOMO: -6.63141 LUMO: -0.88981 factor:1 | 1 (-2.80313) | -1 | -1 |
| G: -2104.18652 HOMO: -7.74164 LUMO: 1.37690 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10475.34959 HOMO: -6.92258 LUMO: -0.82178 factor:1 | 1 (-2.61085) | -1 | -1 |
| G: -2104.18652 HOMO: -7.74164 LUMO: 1.37690 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10475.32080 HOMO: -6.55794 LUMO: -0.80818 factor:1 | 1 (-2.58206) | -1 | -1 |
| G: -2104.18652 HOMO: -7.74164 LUMO: 1.37690 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10475.56559 HOMO: -6.95251 LUMO: -0.97145 factor:1 | 1 (-2.82685) | -1 | -1 |
| G: -2104.18652 HOMO: -7.74164 LUMO: 1.37690 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10476.04312 HOMO: -7.37701 LUMO: 0.14150 factor:1 | 1 (-3.30439) | -1 | -1 |
| G: -2104.18652 HOMO: -7.74164 LUMO: 1.37690 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10475.47204 HOMO: -6.74842 LUMO: -0.68028 factor:1 | 1 (-2.73330) | -1 | -1 |
| G: -2104.18652 HOMO: -7.74164 LUMO: 1.37690 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10475.20499 HOMO: -6.65046 LUMO: -0.52518 factor:1 | 1 (-2.46625) | -1 | -1 |
| G: -2104.18652 HOMO: -7.74164 LUMO: 1.37690 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10475.40363 HOMO: -6.91441 LUMO: -1.13199 factor:1 | 1 (-2.66489) | -1 | -1 |
| G: -2104.18652 HOMO: -7.74164 LUMO: 1.37690 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10475.54771 HOMO: -7.00965 LUMO: -1.00682 factor:1 | 1 (-2.80898) | -1 | -1 |
| G: -2104.18652 HOMO: -7.74164 LUMO: 1.37690 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10475.44760 HOMO: -6.55794 LUMO: -0.54967 factor:1 | 1 (-2.70887) | -1 | -1 |
| G: -2104.18652 HOMO: -7.74164 LUMO: 1.37690 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10475.33829 HOMO: -6.71577 LUMO: -0.53879 factor:1 | 1 (-2.59956) | -1 | -1 |
| G: -2104.18652 HOMO: -7.74164 LUMO: 1.37690 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10475.56799 HOMO: -6.88992 LUMO: -0.55511 factor:1 | 1 (-2.82925) | -1 | -1 |
| G: -2104.18652 HOMO: -7.74164 LUMO: 1.37690 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10475.60178 HOMO: -6.74026 LUMO: -0.60681 factor:1 | 1 (-2.86305) | -1 | -1 |
| G: -2104.18652 HOMO: -7.74164 LUMO: 1.37690 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10475.60064 HOMO: -6.76747 LUMO: -0.50885 factor:1 | 1 (-2.86190) | -1 | -1 |
| G: -2104.18652 HOMO: -7.74164 LUMO: 1.37690 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10475.72377 HOMO: -6.87904 LUMO: -0.92519 factor:1 | 1 (-2.98503) | -1 | -1 |
| G: -2104.18652 HOMO: -7.74164 LUMO: 1.37690 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10475.37568 HOMO: -6.53073 LUMO: -0.53062 factor:1 | 1 (-2.63695) | -1 | -1 |
| G: -2104.18652 HOMO: -7.74164 LUMO: 1.37690 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10475.50828 HOMO: -6.97700 LUMO: -0.98505 factor:1 | 1 (-2.76955) | -1 | -1 |
| G: -2104.18652 HOMO: -7.74164 LUMO: 1.37690 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10475.75237 HOMO: -6.96884 LUMO: -0.79185 factor:1 | 1 (-3.01363) | -1 | -1 |
| G: -2104.18652 HOMO: -7.74164 LUMO: 1.37690 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10475.85275 HOMO: -6.60420 LUMO: -0.31021 factor:1 | 1 (-3.11402) | -1 | -1 |
| G: -2104.18652 HOMO: -7.74164 LUMO: 1.37690 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10475.85828 HOMO: -6.68584 LUMO: -0.63947 factor:1 | 1 (-3.11954) | -1 | -1 |
| G: -2104.18652 HOMO: -7.74164 LUMO: 1.37690 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10475.61645 HOMO: -6.41917 LUMO: -0.35103 factor:1 | 1 (-2.87771) | -1 | -1 |
| G: -2104.18652 HOMO: -7.74164 LUMO: 1.37690 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10475.39125 HOMO: -6.73482 LUMO: -0.70477 factor:1 | 1 (-2.65251) | -1 | -1 |
| G: -2104.18652 HOMO: -7.74164 LUMO: 1.37690 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10475.51604 HOMO: -6.71305 LUMO: -0.85716 factor:1 | 1 (-2.77730) | -1 | -1 |
| G: -2104.18652 HOMO: -7.74164 LUMO: 1.37690 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10475.94182 HOMO: -6.70761 LUMO: -0.63403 factor:1 | 1 (-3.20308) | -1 | -1 |
| G: -2104.18652 HOMO: -7.74164 LUMO: 1.37690 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10476.00443 HOMO: -6.37563 LUMO: -0.38640 factor:1 | 1 (-3.26569) | -1 | -1 |
| G: -2104.18652 HOMO: -7.74164 LUMO: 1.37690 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10476.47323 HOMO: -6.27495 LUMO: -0.54967 factor:1 | 1 (-3.73449) | -1 | -1 |
| G: -2104.18652 HOMO: -7.74164 LUMO: 1.37690 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10477.09601 HOMO: -6.98516 LUMO: 0.38096 factor:1 | 1 (-4.35728) | -1 | -1 |
| G: -2104.18652 HOMO: -7.74164 LUMO: 1.37690 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10476.66918 HOMO: -6.47087 LUMO: -0.40001 factor:1 | 1 (-3.93044) | -1 | -1 |
| G: -2104.18652 HOMO: -7.74164 LUMO: 1.37690 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10475.77468 HOMO: -6.59876 LUMO: 0.20681 factor:1 | 1 (-3.03595) | -1 | -1 |
| G: -2104.18652 HOMO: -7.74164 LUMO: 1.37690 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10475.82791 HOMO: -6.89809 LUMO: 0.14966 factor:1 | 1 (-3.08917) | -1 | -1 |
| G: -2104.18652 HOMO: -7.74164 LUMO: 1.37690 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10474.22616 HOMO: -6.76203 LUMO: 2.11432 factor:1 | 1 (-1.48743) | -1 | -1 |
| G: -2104.18652 HOMO: -7.74164 LUMO: 1.37690 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10474.17890 HOMO: -6.58516 LUMO: 1.75786 factor:1 | 1 (-1.44016) | -1 | -1 |
| G: -2104.18652 HOMO: -7.74164 LUMO: 1.37690 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10473.98325 HOMO: -6.37835 LUMO: 1.84493 factor:1 | 1 (-1.24451) | -1 | -1 |
| G: -2104.18652 HOMO: -7.74164 LUMO: 1.37690 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10474.85045 HOMO: -6.83550 LUMO: 1.74425 factor:1 | 1 (-2.11171) | -1 | -1 |
| G: -2104.18652 HOMO: -7.74164 LUMO: 1.37690 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10474.66827 HOMO: -6.65318 LUMO: 1.79051 factor:1 | 1 (-1.92953) | -1 | -1 |
| G: -2104.18652 HOMO: -7.74164 LUMO: 1.37690 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10474.86011 HOMO: -6.68584 LUMO: 2.11160 factor:1 | 1 (-2.12137) | -1 | -1 |
| G: -2104.18652 HOMO: -7.74164 LUMO: 1.37690 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10474.66427 HOMO: -6.36202 LUMO: 1.85037 factor:1 | 1 (-1.92553) | -1 | -1 |
| G: -2104.18652 HOMO: -7.74164 LUMO: 1.37690 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10474.86890 HOMO: -6.68312 LUMO: 2.23133 factor:1 | 1 (-2.13016) | -1 | -1 |
| G: -2104.18652 HOMO: -7.74164 LUMO: 1.37690 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10474.60617 HOMO: -6.66679 LUMO: 2.14154 factor:1 | 1 (-1.86744) | -1 | -1 |
| G: -2104.18652 HOMO: -7.74164 LUMO: 1.37690 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10474.49861 HOMO: -6.50896 LUMO: 1.92657 factor:1 | 1 (-1.75987) | -1 | -1 |
| G: -2104.18652 HOMO: -7.74164 LUMO: 1.37690 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10474.39547 HOMO: -6.63686 LUMO: 2.22317 factor:1 | 1 (-1.65674) | -1 | -1 |
| G: -2104.18652 HOMO: -7.74164 LUMO: 1.37690 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10474.36837 HOMO: -6.58788 LUMO: 2.17419 factor:1 | 1 (-1.62964) | -1 | -1 |
| G: -2104.18652 HOMO: -7.74164 LUMO: 1.37690 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10474.44922 HOMO: -6.72665 LUMO: 2.12249 factor:1 | 1 (-1.71048) | -1 | -1 |
| G: -2104.18652 HOMO: -7.74164 LUMO: 1.37690 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10475.11154 HOMO: -6.28311 LUMO: 1.91024 factor:1 | 1 (-2.37281) | -1 | -1 |
| G: -2104.18652 HOMO: -7.74164 LUMO: 1.37690 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10475.13451 HOMO: -6.56067 LUMO: 2.27487 factor:1 | 1 (-2.39577) | -1 | -1 |
| G: -2104.18652 HOMO: -7.74164 LUMO: 1.37690 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10475.24561 HOMO: -6.83006 LUMO: 2.28031 factor:1 | 1 (-2.50688) | -1 | -1 |
| G: -2104.18652 HOMO: -7.74164 LUMO: 1.37690 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10474.90073 HOMO: -6.45182 LUMO: 1.62724 factor:1 | 1 (-2.16200) | -1 | -1 |
| G: -2104.18652 HOMO: -7.74164 LUMO: 1.37690 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10475.27160 HOMO: -6.78380 LUMO: 1.83677 factor:1 | 1 (-2.53286) | -1 | -1 |
| G: -2104.18652 HOMO: -7.74164 LUMO: 1.37690 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10475.27367 HOMO: -6.23413 LUMO: 1.80956 factor:1 | 1 (-2.53493) | -1 | -1 |
| G: -2104.18652 HOMO: -7.74164 LUMO: 1.37690 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10475.68704 HOMO: -6.74298 LUMO: 2.16875 factor:1 | 1 (-2.94830) | -1 | -1 |
| G: -2104.18652 HOMO: -7.74164 LUMO: 1.37690 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10475.54654 HOMO: -6.81645 LUMO: 2.50073 factor:1 | 1 (-2.80781) | -1 | -1 |
| G: -2104.18652 HOMO: -7.74164 LUMO: 1.37690 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10475.39443 HOMO: -6.71033 LUMO: 1.96466 factor:1 | 1 (-2.65570) | -1 | -1 |
| G: -2104.18652 HOMO: -7.74164 LUMO: 1.37690 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10475.43032 HOMO: -6.83550 LUMO: 2.04358 factor:1 | 1 (-2.69159) | -1 | -1 |
| G: -2104.18652 HOMO: -7.74164 LUMO: 1.37690 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10476.09567 HOMO: -6.60965 LUMO: 2.38100 factor:1 | 1 (-3.35693) | -1 | -1 |
| G: -2104.18652 HOMO: -7.74164 LUMO: 1.37690 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10476.20296 HOMO: -6.73210 LUMO: 2.26127 factor:1 | 1 (-3.46423) | -1 | -1 |
| G: -2104.18652 HOMO: -7.74164 LUMO: 1.37690 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10476.13798 HOMO: -6.76203 LUMO: 2.13609 factor:1 | 1 (-3.39925) | -1 | -1 |
| G: -2104.18652 HOMO: -7.74164 LUMO: 1.37690 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10475.93863 HOMO: -6.71033 LUMO: 2.05990 factor:1 | 1 (-3.19990) | -1 | -1 |
| G: -2104.18652 HOMO: -7.74164 LUMO: 1.37690 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10475.80989 HOMO: -6.50896 LUMO: 2.32385 factor:1 | 1 (-3.07116) | -1 | -1 |
| G: -2104.18652 HOMO: -7.74164 LUMO: 1.37690 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10475.84943 HOMO: -6.53345 LUMO: 1.74425 factor:1 | 1 (-3.11070) | -1 | -1 |
| G: -2104.18652 HOMO: -7.74164 LUMO: 1.37690 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10474.69246 HOMO: -6.25862 LUMO: 1.63540 factor:1 | 1 (-1.95372) | -1 | -1 |
| G: -2104.18652 HOMO: -7.74164 LUMO: 1.37690 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10474.51654 HOMO: -5.90759 LUMO: 1.78779 factor:1 | 1 (-1.77780) | -1 | -1 |
| G: -2104.18652 HOMO: -7.74164 LUMO: 1.37690 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10474.54851 HOMO: -6.09807 LUMO: 1.99732 factor:1 | 1 (-1.80977) | -1 | -1 |
| G: -2104.18652 HOMO: -7.74164 LUMO: 1.37690 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10474.62204 HOMO: -5.92392 LUMO: 1.99732 factor:1 | 1 (-1.88330) | -1 | -1 |
| G: -2104.18652 HOMO: -7.74164 LUMO: 1.37690 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10474.87540 HOMO: -6.45182 LUMO: 1.72248 factor:1 | 1 (-2.13667) | -1 | -1 |
| G: -2104.18652 HOMO: -7.74164 LUMO: 1.37690 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10474.83496 HOMO: -6.53073 LUMO: 1.82588 factor:1 | 1 (-2.09623) | -1 | -1 |
| G: -2104.18652 HOMO: -7.74164 LUMO: 1.37690 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10474.82645 HOMO: -6.40828 LUMO: 2.05174 factor:1 | 1 (-2.08771) | -1 | -1 |
| G: -2104.18652 HOMO: -7.74164 LUMO: 1.37690 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10475.57571 HOMO: -6.60420 LUMO: -0.82450 factor:1 | 1 (-2.83698) | -1 | -1 |
| G: -2104.18652 HOMO: -7.74164 LUMO: 1.37690 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10475.31682 HOMO: -6.76747 LUMO: -0.57144 factor:1 | 1 (-2.57809) | -1 | -1 |
| G: -2104.18652 HOMO: -7.74164 LUMO: 1.37690 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10475.43740 HOMO: -6.67767 LUMO: -0.59321 factor:1 | 1 (-2.69866) | -1 | -1 |
| G: -2104.18652 HOMO: -7.74164 LUMO: 1.37690 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10476.17855 HOMO: -6.65863 LUMO: -0.57416 factor:1 | 1 (-3.43982) | -1 | -1 |
| G: -2104.18652 HOMO: -7.74164 LUMO: 1.37690 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10476.23249 HOMO: -6.49808 LUMO: -0.54695 factor:1 | 1 (-3.49375) | -1 | -1 |
| G: -2104.18652 HOMO: -7.74164 LUMO: 1.37690 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10476.10617 HOMO: -6.50080 LUMO: -0.61498 factor:1 | 1 (-3.36744) | -1 | -1 |
| G: -2104.18652 HOMO: -7.74164 LUMO: 1.37690 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10476.25532 HOMO: -6.74842 LUMO: -0.51974 factor:1 | 1 (-3.51658) | -1 | -1 |
| G: -2104.18652 HOMO: -7.74164 LUMO: 1.37690 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10475.67182 HOMO: -6.13345 LUMO: 0.67756 factor:1 | 1 (-2.93309) | -1 | -1 |
| G: -2104.18652 HOMO: -7.74164 LUMO: 1.37690 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10475.78124 HOMO: -6.48719 LUMO: 0.52790 factor:1 | 1 (-3.04251) | -1 | -1 |
| G: -2104.18652 HOMO: -7.74164 LUMO: 1.37690 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10475.76957 HOMO: -6.35930 LUMO: 0.74015 factor:1 | 1 (-3.03083) | -1 | -1 |
| G: -2104.18652 HOMO: -7.74164 LUMO: 1.37690 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10475.75841 HOMO: -6.41644 LUMO: 0.22313 factor:1 | 1 (-3.01967) | -1 | -1 |
| G: -2104.18652 HOMO: -7.74164 LUMO: 1.37690 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10475.48959 HOMO: -6.85727 LUMO: -0.00272 factor:1 | 1 (-2.75085) | -1 | -1 |
| G: -2104.18652 HOMO: -7.74164 LUMO: 1.37690 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10475.73953 HOMO: -6.84638 LUMO: 0.24762 factor:1 | 1 (-3.00079) | -1 | -1 |
| G: -2104.18652 HOMO: -7.74164 LUMO: 1.37690 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10475.67354 HOMO: -6.66951 LUMO: 0.39184 factor:1 | 1 (-2.93480) | -1 | -1 |
| G: -2104.18652 HOMO: -7.74164 LUMO: 1.37690 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10476.45078 HOMO: -6.62597 LUMO: -0.65035 factor:1 | 1 (-3.71204) | -1 | -1 |
| G: -2104.18652 HOMO: -7.74164 LUMO: 1.37690 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10477.32720 HOMO: -7.13755 LUMO: 0.45715 factor:1 | 1 (-4.58847) | -1 | -1 |
| G: -2104.18652 HOMO: -7.74164 LUMO: 1.37690 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10477.19890 HOMO: -7.12666 LUMO: 0.45171 factor:1 | 1 (-4.46016) | -1 | -1 |
| G: -2104.18652 HOMO: -7.74164 LUMO: 1.37690 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10476.35858 HOMO: -6.46270 LUMO: -0.46259 factor:1 | 1 (-3.61985) | -1 | -1 |
| G: -2104.18652 HOMO: -7.74164 LUMO: 1.37690 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10476.52623 HOMO: -6.36202 LUMO: -0.29660 factor:1 | 1 (-3.78750) | -1 | -1 |
| G: -2104.18652 HOMO: -7.74164 LUMO: 1.37690 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10475.81166 HOMO: -6.28583 LUMO: 0.40545 factor:1 | 1 (-3.07293) | -1 | -1 |
| G: -2104.18652 HOMO: -7.74164 LUMO: 1.37690 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10475.80059 HOMO: -6.70761 LUMO: 0.41906 factor:1 | 1 (-3.06185) | -1 | -1 |
| G: -2104.18652 HOMO: -7.74164 LUMO: 1.37690 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10475.35296 HOMO: -6.76203 LUMO: -0.60954 factor:1 | 1 (-2.61423) | -1 | -1 |
| G: -2104.18652 HOMO: -7.74164 LUMO: 1.37690 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10475.23462 HOMO: -6.85999 LUMO: -0.75103 factor:1 | 1 (-2.49588) | -1 | -1 |
| G: -2104.18652 HOMO: -7.74164 LUMO: 1.37690 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10475.50744 HOMO: -7.19741 LUMO: -1.00954 factor:1 | 1 (-2.76870) | -1 | -1 |
| G: -2104.18652 HOMO: -7.74164 LUMO: 1.37690 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10475.71090 HOMO: -6.58243 LUMO: -0.33470 factor:1 | 1 (-2.97216) | -1 | -1 |
| G: -2104.18652 HOMO: -7.74164 LUMO: 1.37690 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10476.39358 HOMO: -7.22190 LUMO: 0.49253 factor:1 | 1 (-3.65484) | -1 | -1 |
| G: -2104.18652 HOMO: -7.74164 LUMO: 1.37690 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10476.31116 HOMO: -7.22462 LUMO: 0.51974 factor:1 | 1 (-3.57242) | -1 | -1 |
| G: -2104.18652 HOMO: -7.74164 LUMO: 1.37690 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10475.70440 HOMO: -7.08584 LUMO: -0.68301 factor:1 | 1 (-2.96566) | -1 | -1 |
| G: -2104.18652 HOMO: -7.74164 LUMO: 1.37690 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10475.77849 HOMO: -6.68584 LUMO: -0.29660 factor:1 | 1 (-3.03976) | -1 | -1 |
| G: -2104.18652 HOMO: -7.74164 LUMO: 1.37690 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10475.40567 HOMO: -6.33753 LUMO: -0.48436 factor:1 | 1 (-2.66693) | -1 | -1 |
| G: -2104.18652 HOMO: -7.74164 LUMO: 1.37690 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10476.45785 HOMO: -7.15932 LUMO: 0.55511 factor:1 | 1 (-3.71912) | -1 | -1 |
| G: -2104.18652 HOMO: -7.74164 LUMO: 1.37690 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10473.70079 HOMO: -6.57427 LUMO: 2.01908 factor:1 | 1 (-0.96206) | -1 | -1 |
| G: -2104.18652 HOMO: -7.74164 LUMO: 1.37690 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10474.00845 HOMO: -6.75659 LUMO: 2.22045 factor:1 | 1 (-1.26971) | -1 | -1 |
| G: -2104.18652 HOMO: -7.74164 LUMO: 1.37690 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10473.91073 HOMO: -6.73482 LUMO: 2.20956 factor:1 | 1 (-1.17199) | -1 | -1 |
| G: -2104.18652 HOMO: -7.74164 LUMO: 1.37690 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10473.97277 HOMO: -6.74026 LUMO: 1.76602 factor:1 | 1 (-1.23404) | -1 | -1 |
| G: -2104.18652 HOMO: -7.74164 LUMO: 1.37690 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10474.60998 HOMO: -6.95523 LUMO: 1.94834 factor:1 | 1 (-1.87125) | -1 | -1 |
| G: -2104.18652 HOMO: -7.74164 LUMO: 1.37690 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10474.42511 HOMO: -6.33209 LUMO: 1.87486 factor:1 | 1 (-1.68637) | -1 | -1 |
| G: -2104.18652 HOMO: -7.74164 LUMO: 1.37690 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10474.76441 HOMO: -6.71033 LUMO: 2.12521 factor:1 | 1 (-2.02567) | -1 | -1 |
| G: -2104.18652 HOMO: -7.74164 LUMO: 1.37690 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10474.33566 HOMO: -6.50080 LUMO: 2.04902 factor:1 | 1 (-1.59693) | -1 | -1 |
| G: -2104.18652 HOMO: -7.74164 LUMO: 1.37690 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10474.57395 HOMO: -6.76475 LUMO: 1.94017 factor:1 | 1 (-1.83522) | -1 | -1 |
| G: -2104.18652 HOMO: -7.74164 LUMO: 1.37690 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10474.61406 HOMO: -6.53073 LUMO: 2.08983 factor:1 | 1 (-1.87533) | -1 | -1 |
| G: -2104.18652 HOMO: -7.74164 LUMO: 1.37690 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10474.93649 HOMO: -6.69944 LUMO: 2.20684 factor:1 | 1 (-2.19775) | -1 | -1 |
| G: -2104.18652 HOMO: -7.74164 LUMO: 1.37690 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10474.77586 HOMO: -6.34570 LUMO: 1.80684 factor:1 | 1 (-2.03713) | -1 | -1 |
| G: -2104.18652 HOMO: -7.74164 LUMO: 1.37690 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10475.04381 HOMO: -6.78380 LUMO: 1.95922 factor:1 | 1 (-2.30508) | -1 | -1 |
| G: -2104.18652 HOMO: -7.74164 LUMO: 1.37690 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10474.69006 HOMO: -6.93618 LUMO: 1.76058 factor:1 | 1 (-1.95133) | -1 | -1 |
| G: -2104.18652 HOMO: -7.74164 LUMO: 1.37690 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10474.75295 HOMO: -6.93346 LUMO: 1.79595 factor:1 | 1 (-2.01421) | -1 | -1 |
| G: -2104.18652 HOMO: -7.74164 LUMO: 1.37690 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10474.75355 HOMO: -6.29671 LUMO: 1.75241 factor:1 | 1 (-2.01481) | -1 | -1 |
| G: -2104.18652 HOMO: -7.74164 LUMO: 1.37690 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10474.73964 HOMO: -6.77019 LUMO: 1.74697 factor:1 | 1 (-2.00091) | -1 | -1 |
| G: -2104.18652 HOMO: -7.74164 LUMO: 1.37690 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10474.41945 HOMO: -6.87360 LUMO: 1.91024 factor:1 | 1 (-1.68071) | -1 | -1 |
| G: -2104.18652 HOMO: -7.74164 LUMO: 1.37690 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10474.61085 HOMO: -6.32665 LUMO: 1.87759 factor:1 | 1 (-1.87212) | -1 | -1 |
| G: -2104.18652 HOMO: -7.74164 LUMO: 1.37690 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10474.56470 HOMO: -6.99877 LUMO: 1.99187 factor:1 | 1 (-1.82597) | -1 | -1 |
| G: -2104.18652 HOMO: -7.74164 LUMO: 1.37690 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10475.27734 HOMO: -6.72665 LUMO: 2.12521 factor:1 | 1 (-2.53860) | -1 | -1 |
| G: -2104.18652 HOMO: -7.74164 LUMO: 1.37690 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10475.41416 HOMO: -6.67767 LUMO: 2.43814 factor:1 | 1 (-2.67542) | -1 | -1 |
| G: -2104.18652 HOMO: -7.74164 LUMO: 1.37690 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10475.37261 HOMO: -6.99605 LUMO: 1.79051 factor:1 | 1 (-2.63387) | -1 | -1 |
| G: -2104.18652 HOMO: -7.74164 LUMO: 1.37690 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10475.19372 HOMO: -6.25046 LUMO: 1.77146 factor:1 | 1 (-2.45498) | -1 | -1 |
| G: -2104.18652 HOMO: -7.74164 LUMO: 1.37690 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10474.44519 HOMO: -6.30488 LUMO: 1.90480 factor:1 | 1 (-1.70645) | -1 | -1 |
| G: -2104.18652 HOMO: -7.74164 LUMO: 1.37690 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10474.42995 HOMO: -6.38379 LUMO: 1.68438 factor:1 | 1 (-1.69121) | -1 | -1 |
| G: -2104.18652 HOMO: -7.74164 LUMO: 1.37690 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10474.79192 HOMO: -6.78924 LUMO: 2.01364 factor:1 | 1 (-2.05318) | -1 | -1 |
| G: -2104.18652 HOMO: -7.74164 LUMO: 1.37690 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10474.46805 HOMO: -6.15249 LUMO: 1.98643 factor:1 | 1 (-1.72931) | -1 | -1 |
| G: -2104.18652 HOMO: -7.74164 LUMO: 1.37690 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10474.19604 HOMO: -6.19331 LUMO: 2.14154 factor:1 | 1 (-1.45731) | -1 | -1 |
| G: -2104.18652 HOMO: -7.74164 LUMO: 1.37690 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10474.32818 HOMO: -6.05998 LUMO: 2.12521 factor:1 | 1 (-1.58944) | -1 | -1 |
| G: -2104.18652 HOMO: -7.74164 LUMO: 1.37690 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10474.56212 HOMO: -6.67223 LUMO: 1.91840 factor:1 | 1 (-1.82338) | -1 | -1 |
| G: -2104.18652 HOMO: -7.74164 LUMO: 1.37690 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10474.73483 HOMO: -6.79196 LUMO: 2.18507 factor:1 | 1 (-1.99609) | -1 | -1 |
| G: -2104.18652 HOMO: -7.74164 LUMO: 1.37690 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10474.70566 HOMO: -6.93346 LUMO: 1.78235 factor:1 | 1 (-1.96692) | -1 | -1 |
| G: -2104.18652 HOMO: -7.74164 LUMO: 1.37690 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10474.67093 HOMO: -6.16882 LUMO: 1.80956 factor:1 | 1 (-1.93220) | -1 | -1 |
| G: -2104.18652 HOMO: -7.74164 LUMO: 1.37690 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10474.65298 HOMO: -6.72665 LUMO: 2.07895 factor:1 | 1 (-1.91424) | -1 | -1 |
| G: -2104.18652 HOMO: -7.74164 LUMO: 1.37690 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10474.72081 HOMO: -6.73210 LUMO: 1.97827 factor:1 | 1 (-1.98208) | -1 | -1 |
| G: -2104.18652 HOMO: -7.74164 LUMO: 1.37690 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10474.62133 HOMO: -6.84638 LUMO: 1.87214 factor:1 | 1 (-1.88259) | -1 | -1 |
| G: -2104.18652 HOMO: -7.74164 LUMO: 1.37690 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10475.42804 HOMO: -6.83006 LUMO: 2.36195 factor:1 | 1 (-2.68930) | -1 | -1 |
| G: -2104.18652 HOMO: -7.74164 LUMO: 1.37690 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10475.58037 HOMO: -6.97700 LUMO: 1.91024 factor:1 | 1 (-2.84163) | -1 | -1 |
| G: -2104.18652 HOMO: -7.74164 LUMO: 1.37690 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10475.19173 HOMO: -6.20420 LUMO: 1.81772 factor:1 | 1 (-2.45300) | -1 | -1 |
| G: -2104.18652 HOMO: -7.74164 LUMO: 1.37690 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10474.67610 HOMO: -7.09129 LUMO: 2.10344 factor:1 | 1 (-1.93737) | 1 | 1 |
| G: -2104.18652 HOMO: -7.74164 LUMO: 1.37690 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10474.58838 HOMO: -6.77564 LUMO: 2.14970 factor:1 | 1 (-1.84964) | -1 | -1 |
| G: -2104.18652 HOMO: -7.74164 LUMO: 1.37690 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10474.38513 HOMO: -6.81645 LUMO: 1.85854 factor:1 | 1 (-1.64640) | -1 | -1 |
| G: -2104.18652 HOMO: -7.74164 LUMO: 1.37690 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10474.43879 HOMO: -6.50896 LUMO: 2.04358 factor:1 | 1 (-1.70006) | -1 | -1 |
| G: -2104.18652 HOMO: -7.74164 LUMO: 1.37690 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10474.53469 HOMO: -6.89264 LUMO: 1.66262 factor:1 | 1 (-1.79595) | -1 | -1 |
| G: -2104.18652 HOMO: -7.74164 LUMO: 1.37690 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10474.19737 HOMO: -6.75931 LUMO: 2.23950 factor:1 | 1 (-1.45864) | -1 | -1 |
| G: -2104.18652 HOMO: -7.74164 LUMO: 1.37690 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10474.55262 HOMO: -6.50080 LUMO: 1.67622 factor:1 | 1 (-1.81388) | -1 | -1 |
| G: -2104.18652 HOMO: -7.74164 LUMO: 1.37690 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10474.63137 HOMO: -6.30216 LUMO: 2.24222 factor:1 | 1 (-1.89263) | -1 | -1 |
| G: -2104.18652 HOMO: -7.74164 LUMO: 1.37690 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10474.62663 HOMO: -7.18108 LUMO: 2.10072 factor:1 | 1 (-1.88790) | 1 | 1 |
| G: -2104.18652 HOMO: -7.74164 LUMO: 1.37690 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10474.71409 HOMO: -6.54162 LUMO: 2.35378 factor:1 | 1 (-1.97536) | -1 | -1 |
| G: -2104.18652 HOMO: -7.74164 LUMO: 1.37690 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10474.48976 HOMO: -5.98650 LUMO: 1.48302 factor:1 | 1 (-1.75103) | -1 | -1 |
| G: -2104.18652 HOMO: -7.74164 LUMO: 1.37690 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10474.52252 HOMO: -7.15115 LUMO: 2.14970 factor:1 | 1 (-1.78379) | 1 | 1 |
| G: -2104.18652 HOMO: -7.74164 LUMO: 1.37690 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10474.55142 HOMO: -6.45454 LUMO: 2.15786 factor:1 | 1 (-1.81269) | -1 | -1 |
| G: -2104.18652 HOMO: -7.74164 LUMO: 1.37690 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10474.62383 HOMO: -7.06952 LUMO: 2.14970 factor:1 | 1 (-1.88510) | 1 | 1 |
| G: -2104.18652 HOMO: -7.74164 LUMO: 1.37690 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10474.67314 HOMO: -6.93618 LUMO: 1.86942 factor:1 | 1 (-1.93440) | -1 | -1 |
| G: -2104.18652 HOMO: -7.74164 LUMO: 1.37690 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10474.61477 HOMO: -6.63141 LUMO: 1.92657 factor:1 | 1 (-1.87603) | -1 | -1 |
| G: -2104.18652 HOMO: -7.74164 LUMO: 1.37690 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10475.53917 HOMO: -6.51441 LUMO: -0.44355 factor:1 | 1 (-2.80043) | -1 | -1 |
| G: -2104.18652 HOMO: -7.74164 LUMO: 1.37690 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10475.68535 HOMO: -6.82734 LUMO: -1.03131 factor:1 | 1 (-2.94661) | -1 | -1 |
| G: -2104.18652 HOMO: -7.74164 LUMO: 1.37690 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10475.49503 HOMO: -6.58788 LUMO: -0.82995 factor:1 | 1 (-2.75630) | -1 | -1 |
| G: -2104.18652 HOMO: -7.74164 LUMO: 1.37690 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10475.80315 HOMO: -6.43277 LUMO: -0.40817 factor:1 | 1 (-3.06441) | -1 | -1 |
| G: -2104.18652 HOMO: -7.74164 LUMO: 1.37690 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10475.88799 HOMO: -6.78924 LUMO: -0.72110 factor:1 | 1 (-3.14926) | -1 | -1 |
| G: -2104.18652 HOMO: -7.74164 LUMO: 1.37690 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10476.78956 HOMO: -7.28177 LUMO: 0.36735 factor:1 | 1 (-4.05082) | -1 | -1 |
| G: -2104.18652 HOMO: -7.74164 LUMO: 1.37690 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10475.67846 HOMO: -6.47903 LUMO: -0.46259 factor:1 | 1 (-2.93973) | -1 | -1 |
| G: -2104.18652 HOMO: -7.74164 LUMO: 1.37690 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10475.95093 HOMO: -6.67495 LUMO: -0.75376 factor:1 | 1 (-3.21220) | -1 | -1 |
| G: -2104.18652 HOMO: -7.74164 LUMO: 1.37690 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10475.91422 HOMO: -6.71033 LUMO: -0.71838 factor:1 | 1 (-3.17549) | -1 | -1 |
| G: -2104.18652 HOMO: -7.74164 LUMO: 1.37690 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10475.95493 HOMO: -6.79740 LUMO: -0.79185 factor:1 | 1 (-3.21620) | -1 | -1 |
| G: -2104.18652 HOMO: -7.74164 LUMO: 1.37690 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10475.62878 HOMO: -6.08719 LUMO: -0.63675 factor:1 | 1 (-2.89004) | -1 | -1 |
| G: -2104.18652 HOMO: -7.74164 LUMO: 1.37690 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10475.99110 HOMO: -6.84094 LUMO: 0.42994 factor:1 | 1 (-3.25236) | -1 | -1 |
| G: -2104.18652 HOMO: -7.74164 LUMO: 1.37690 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10475.78263 HOMO: -6.59604 LUMO: 0.25851 factor:1 | 1 (-3.04389) | -1 | -1 |
| G: -2104.18652 HOMO: -7.74164 LUMO: 1.37690 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10475.99463 HOMO: -6.82462 LUMO: 0.08708 factor:1 | 1 (-3.25590) | -1 | -1 |
| G: -2104.18652 HOMO: -7.74164 LUMO: 1.37690 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10475.81613 HOMO: -6.54706 LUMO: 0.44082 factor:1 | 1 (-3.07739) | -1 | -1 |
| G: -2104.18652 HOMO: -7.74164 LUMO: 1.37690 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10477.08548 HOMO: -6.99333 LUMO: 0.32109 factor:1 | 1 (-4.34675) | -1 | -1 |
| G: -2104.18652 HOMO: -7.74164 LUMO: 1.37690 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10476.37146 HOMO: -6.29944 LUMO: -0.57144 factor:1 | 1 (-3.63272) | -1 | -1 |
| G: -2104.18652 HOMO: -7.74164 LUMO: 1.37690 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10476.48313 HOMO: -6.57699 LUMO: -0.46531 factor:1 | 1 (-3.74440) | -1 | -1 |
| G: -2104.18652 HOMO: -7.74164 LUMO: 1.37690 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10476.48036 HOMO: -6.24773 LUMO: -0.53879 factor:1 | 1 (-3.74162) | -1 | -1 |
| G: -2104.18652 HOMO: -7.74164 LUMO: 1.37690 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10476.80303 HOMO: -6.96067 LUMO: -0.67212 factor:1 | 1 (-4.06429) | -1 | -1 |
| G: -2104.18652 HOMO: -7.74164 LUMO: 1.37690 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10476.70904 HOMO: -7.24095 LUMO: -0.09252 factor:1 | 1 (-3.97030) | -1 | -1 |
| G: -2104.18652 HOMO: -7.74164 LUMO: 1.37690 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10476.12288 HOMO: -6.33481 LUMO: -0.46531 factor:1 | 1 (-3.38414) | -1 | -1 |
| G: -2104.18652 HOMO: -7.74164 LUMO: 1.37690 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10476.22617 HOMO: -6.43549 LUMO: -0.33198 factor:1 | 1 (-3.48744) | -1 | -1 |
| G: -2104.18652 HOMO: -7.74164 LUMO: 1.37690 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10475.50948 HOMO: -6.53073 LUMO: 0.44899 factor:1 | 1 (-2.77074) | -1 | -1 |
| G: -2104.18652 HOMO: -7.74164 LUMO: 1.37690 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10475.60584 HOMO: -6.69128 LUMO: 0.47620 factor:1 | 1 (-2.86710) | -1 | -1 |
| G: -2104.18652 HOMO: -7.74164 LUMO: 1.37690 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10475.42001 HOMO: -6.65318 LUMO: 0.52246 factor:1 | 1 (-2.68127) | -1 | -1 |
| G: -2104.18652 HOMO: -7.74164 LUMO: 1.37690 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10475.50050 HOMO: -6.71305 LUMO: 0.41089 factor:1 | 1 (-2.76177) | -1 | -1 |
| G: -2104.18652 HOMO: -7.74164 LUMO: 1.37690 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10475.38978 HOMO: -6.70216 LUMO: 0.19864 factor:1 | 1 (-2.65104) | -1 | -1 |
| G: -2104.18652 HOMO: -7.74164 LUMO: 1.37690 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10475.41832 HOMO: -6.41100 LUMO: 0.34558 factor:1 | 1 (-2.67959) | -1 | -1 |
| G: -2104.18652 HOMO: -7.74164 LUMO: 1.37690 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10475.73261 HOMO: -7.01237 LUMO: 0.02993 factor:1 | 1 (-2.99388) | -1 | -1 |
| G: -2104.18652 HOMO: -7.74164 LUMO: 1.37690 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10475.84489 HOMO: -6.85999 LUMO: 0.18776 factor:1 | 1 (-3.10615) | -1 | -1 |
| G: -2104.18652 HOMO: -7.74164 LUMO: 1.37690 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10476.04574 HOMO: -6.62869 LUMO: 0.48708 factor:1 | 1 (-3.30700) | -1 | -1 |
| G: -2104.18652 HOMO: -7.74164 LUMO: 1.37690 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10476.58621 HOMO: -6.43821 LUMO: -0.45715 factor:1 | 1 (-3.84747) | -1 | -1 |
| G: -2104.18652 HOMO: -7.74164 LUMO: 1.37690 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10476.57067 HOMO: -6.43277 LUMO: -0.72110 factor:1 | 1 (-3.83193) | -1 | -1 |
| G: -2104.18652 HOMO: -7.74164 LUMO: 1.37690 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10477.21316 HOMO: -7.10761 LUMO: 0.43266 factor:1 | 1 (-4.47442) | -1 | -1 |
| G: -2104.18652 HOMO: -7.74164 LUMO: 1.37690 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10476.46240 HOMO: -6.57699 LUMO: -0.61498 factor:1 | 1 (-3.72366) | -1 | -1 |
| G: -2104.18652 HOMO: -7.74164 LUMO: 1.37690 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10476.64991 HOMO: -6.82189 LUMO: -0.75648 factor:1 | 1 (-3.91117) | -1 | -1 |
| G: -2104.18652 HOMO: -7.74164 LUMO: 1.37690 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10476.52607 HOMO: -6.55794 LUMO: -0.67212 factor:1 | 1 (-3.78734) | -1 | -1 |
| G: -2104.18652 HOMO: -7.74164 LUMO: 1.37690 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10474.65148 HOMO: -6.69128 LUMO: 1.88575 factor:1 | 1 (-1.91274) | -1 | -1 |
| G: -2104.18652 HOMO: -7.74164 LUMO: 1.37690 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10474.86065 HOMO: -6.65591 LUMO: 1.70888 factor:1 | 1 (-2.12192) | -1 | -1 |
| G: -2104.18652 HOMO: -7.74164 LUMO: 1.37690 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10474.67776 HOMO: -6.58788 LUMO: 1.68438 factor:1 | 1 (-1.93903) | -1 | -1 |
| G: -2104.18652 HOMO: -7.74164 LUMO: 1.37690 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10474.80204 HOMO: -6.46270 LUMO: 1.72520 factor:1 | 1 (-2.06330) | -1 | -1 |
| G: -2104.18652 HOMO: -7.74164 LUMO: 1.37690 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10474.78974 HOMO: -6.57427 LUMO: 1.73881 factor:1 | 1 (-2.05100) | -1 | -1 |
| G: -2104.18652 HOMO: -7.74164 LUMO: 1.37690 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10474.76941 HOMO: -6.45182 LUMO: 1.75241 factor:1 | 1 (-2.03068) | -1 | -1 |
| G: -2104.18652 HOMO: -7.74164 LUMO: 1.37690 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10474.38372 HOMO: -6.51441 LUMO: 1.78779 factor:1 | 1 (-1.64498) | -1 | -1 |
| G: -2104.18652 HOMO: -7.74164 LUMO: 1.37690 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10474.59744 HOMO: -6.67495 LUMO: 2.11705 factor:1 | 1 (-1.85870) | -1 | -1 |
| G: -2104.18652 HOMO: -7.74164 LUMO: 1.37690 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10474.38407 HOMO: -6.22597 LUMO: 1.96466 factor:1 | 1 (-1.64534) | -1 | -1 |
| G: -2104.18652 HOMO: -7.74164 LUMO: 1.37690 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10474.40184 HOMO: -6.68040 LUMO: 2.30753 factor:1 | 1 (-1.66311) | -1 | -1 |
| G: -2104.18652 HOMO: -7.74164 LUMO: 1.37690 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10474.39937 HOMO: -6.65046 LUMO: 2.18235 factor:1 | 1 (-1.66063) | -1 | -1 |
| G: -2104.18652 HOMO: -7.74164 LUMO: 1.37690 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10474.51167 HOMO: -6.38651 LUMO: 1.76874 factor:1 | 1 (-1.77293) | -1 | -1 |
| G: -2104.18652 HOMO: -7.74164 LUMO: 1.37690 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10475.17154 HOMO: -6.41644 LUMO: 2.09256 factor:1 | 1 (-2.43281) | -1 | -1 |
| G: -2104.18652 HOMO: -7.74164 LUMO: 1.37690 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10474.98267 HOMO: -6.14977 LUMO: 2.28031 factor:1 | 1 (-2.24393) | -1 | -1 |
| G: -2104.18652 HOMO: -7.74164 LUMO: 1.37690 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10475.22583 HOMO: -6.70489 LUMO: 2.43814 factor:1 | 1 (-2.48709) | -1 | -1 |
| G: -2104.18652 HOMO: -7.74164 LUMO: 1.37690 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10475.45789 HOMO: -6.78924 LUMO: 2.27215 factor:1 | 1 (-2.71915) | -1 | -1 |
| G: -2104.18652 HOMO: -7.74164 LUMO: 1.37690 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10475.42385 HOMO: -6.86271 LUMO: 2.31025 factor:1 | 1 (-2.68511) | -1 | -1 |
| G: -2104.18652 HOMO: -7.74164 LUMO: 1.37690 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10475.24041 HOMO: -6.51168 LUMO: 2.04630 factor:1 | 1 (-2.50168) | -1 | -1 |
| G: -2104.18652 HOMO: -7.74164 LUMO: 1.37690 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10475.20373 HOMO: -6.72665 LUMO: 2.13337 factor:1 | 1 (-2.46500) | -1 | -1 |
| G: -2104.18652 HOMO: -7.74164 LUMO: 1.37690 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10475.21701 HOMO: -6.45998 LUMO: 2.16058 factor:1 | 1 (-2.47828) | -1 | -1 |
| G: -2104.18652 HOMO: -7.74164 LUMO: 1.37690 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10475.54575 HOMO: -6.83822 LUMO: 2.20684 factor:1 | 1 (-2.80702) | -1 | -1 |
| G: -2104.18652 HOMO: -7.74164 LUMO: 1.37690 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10475.48265 HOMO: -6.68856 LUMO: 2.19324 factor:1 | 1 (-2.74391) | -1 | -1 |
| G: -2104.18652 HOMO: -7.74164 LUMO: 1.37690 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10475.49310 HOMO: -6.71577 LUMO: 2.16058 factor:1 | 1 (-2.75436) | -1 | -1 |
| G: -2104.18652 HOMO: -7.74164 LUMO: 1.37690 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10475.17138 HOMO: -6.82462 LUMO: 1.90208 factor:1 | 1 (-2.43264) | -1 | -1 |
| G: -2104.18652 HOMO: -7.74164 LUMO: 1.37690 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10475.39702 HOMO: -6.61509 LUMO: 2.23950 factor:1 | 1 (-2.65828) | -1 | -1 |
| G: -2104.18652 HOMO: -7.74164 LUMO: 1.37690 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10475.37742 HOMO: -6.73754 LUMO: 1.84221 factor:1 | 1 (-2.63869) | -1 | -1 |
| G: -2104.18652 HOMO: -7.74164 LUMO: 1.37690 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10475.43468 HOMO: -6.56611 LUMO: 1.94561 factor:1 | 1 (-2.69594) | -1 | -1 |
| G: -2104.18652 HOMO: -7.74164 LUMO: 1.37690 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10475.38899 HOMO: -6.67767 LUMO: 1.51840 factor:1 | 1 (-2.65025) | -1 | -1 |
| G: -2104.18652 HOMO: -7.74164 LUMO: 1.37690 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10475.20311 HOMO: -6.35658 LUMO: 2.16603 factor:1 | 1 (-2.46437) | -1 | -1 |
| G: -2104.18652 HOMO: -7.74164 LUMO: 1.37690 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10475.31941 HOMO: -6.35114 LUMO: 2.08983 factor:1 | 1 (-2.58067) | -1 | -1 |
| G: -2104.18652 HOMO: -7.74164 LUMO: 1.37690 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10475.30817 HOMO: -6.35114 LUMO: 2.10616 factor:1 | 1 (-2.56944) | -1 | -1 |
| G: -2104.18652 HOMO: -7.74164 LUMO: 1.37690 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10475.24637 HOMO: -6.71305 LUMO: 2.01636 factor:1 | 1 (-2.50764) | -1 | -1 |
| G: -2104.18652 HOMO: -7.74164 LUMO: 1.37690 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10475.12866 HOMO: -6.24773 LUMO: 1.98915 factor:1 | 1 (-2.38992) | -1 | -1 |
| G: -2104.18652 HOMO: -7.74164 LUMO: 1.37690 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10475.20474 HOMO: -6.53617 LUMO: 2.42726 factor:1 | 1 (-2.46600) | -1 | -1 |
| G: -2104.18652 HOMO: -7.74164 LUMO: 1.37690 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10475.37127 HOMO: -6.59332 LUMO: 1.82316 factor:1 | 1 (-2.63254) | -1 | -1 |
| G: -2104.18652 HOMO: -7.74164 LUMO: 1.37690 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10474.26475 HOMO: -6.41372 LUMO: 1.77418 factor:1 | 1 (-1.52601) | -1 | -1 |
| G: -2104.18652 HOMO: -7.74164 LUMO: 1.37690 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10474.37659 HOMO: -6.40284 LUMO: 1.88575 factor:1 | 1 (-1.63785) | -1 | -1 |
| G: -2104.18652 HOMO: -7.74164 LUMO: 1.37690 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10474.26527 HOMO: -6.11168 LUMO: 1.70888 factor:1 | 1 (-1.52653) | -1 | -1 |
| G: -2104.18652 HOMO: -7.74164 LUMO: 1.37690 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10474.32530 HOMO: -6.44910 LUMO: 2.23405 factor:1 | 1 (-1.58656) | -1 | -1 |
| G: -2104.18652 HOMO: -7.74164 LUMO: 1.37690 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10474.10687 HOMO: -6.24773 LUMO: 2.12793 factor:1 | 1 (-1.36813) | -1 | -1 |
| G: -2104.18652 HOMO: -7.74164 LUMO: 1.37690 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10474.03996 HOMO: -6.07358 LUMO: 1.89663 factor:1 | 1 (-1.30122) | -1 | -1 |
| G: -2104.18652 HOMO: -7.74164 LUMO: 1.37690 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10474.45303 HOMO: -6.66679 LUMO: 1.96738 factor:1 | 1 (-1.71429) | -1 | -1 |
| G: -2104.18652 HOMO: -7.74164 LUMO: 1.37690 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10474.83611 HOMO: -6.68312 LUMO: 1.78235 factor:1 | 1 (-2.09737) | -1 | -1 |
| G: -2104.18652 HOMO: -7.74164 LUMO: 1.37690 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10474.64737 HOMO: -6.70761 LUMO: 1.97555 factor:1 | 1 (-1.90863) | -1 | -1 |
| G: -2104.18652 HOMO: -7.74164 LUMO: 1.37690 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10474.38941 HOMO: -6.15794 LUMO: 2.00548 factor:1 | 1 (-1.65067) | -1 | -1 |
| G: -2104.18652 HOMO: -7.74164 LUMO: 1.37690 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10474.63610 HOMO: -6.52257 LUMO: 1.96738 factor:1 | 1 (-1.89737) | -1 | -1 |
| G: -2104.18652 HOMO: -7.74164 LUMO: 1.37690 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10474.50971 HOMO: -6.25590 LUMO: 1.86670 factor:1 | 1 (-1.77097) | -1 | -1 |
| G: -2104.18652 HOMO: -7.74164 LUMO: 1.37690 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10475.21522 HOMO: -6.30216 LUMO: 1.84765 factor:1 | 1 (-2.47648) | -1 | -1 |
| G: -2104.18652 HOMO: -7.74164 LUMO: 1.37690 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10475.70573 HOMO: -6.76747 LUMO: 2.20956 factor:1 | 1 (-2.96699) | -1 | -1 |
| G: -2104.18652 HOMO: -7.74164 LUMO: 1.37690 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10475.16855 HOMO: -6.14161 LUMO: 1.80684 factor:1 | 1 (-2.42981) | -1 | -1 |
| G: -2104.18652 HOMO: -7.74164 LUMO: 1.37690 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10475.40344 HOMO: -6.81373 LUMO: 1.91024 factor:1 | 1 (-2.66470) | -1 | -1 |
| G: -2104.18652 HOMO: -7.74164 LUMO: 1.37690 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10475.54192 HOMO: -6.81917 LUMO: 2.34834 factor:1 | 1 (-2.80318) | -1 | -1 |
| G: -2104.18652 HOMO: -7.74164 LUMO: 1.37690 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10475.46137 HOMO: -6.72121 LUMO: 1.90208 factor:1 | 1 (-2.72264) | -1 | -1 |
| G: -2104.18652 HOMO: -7.74164 LUMO: 1.37690 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10476.14976 HOMO: -7.51851 LUMO: 0.26939 factor:1 | 1 (-3.41103) | -1 | -1 |
| G: -2104.18652 HOMO: -7.74164 LUMO: 1.37690 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10475.47922 HOMO: -6.65318 LUMO: -0.57144 factor:1 | 1 (-2.74049) | -1 | -1 |
| G: -2104.18652 HOMO: -7.74164 LUMO: 1.37690 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10475.42532 HOMO: -6.77564 LUMO: -0.72654 factor:1 | 1 (-2.68658) | -1 | -1 |
| G: -2104.18652 HOMO: -7.74164 LUMO: 1.37690 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10475.53367 HOMO: -6.80557 LUMO: -0.60954 factor:1 | 1 (-2.79494) | -1 | -1 |
| G: -2104.18652 HOMO: -7.74164 LUMO: 1.37690 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10476.61886 HOMO: -7.35524 LUMO: 0.27483 factor:1 | 1 (-3.88013) | -1 | -1 |
| G: -2104.18652 HOMO: -7.74164 LUMO: 1.37690 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10475.74524 HOMO: -6.94979 LUMO: -0.83811 factor:1 | 1 (-3.00650) | -1 | -1 |
| G: -2104.18652 HOMO: -7.74164 LUMO: 1.37690 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10475.69939 HOMO: -6.13345 LUMO: -0.67212 factor:1 | 1 (-2.96065) | -1 | -1 |
| G: -2104.18652 HOMO: -7.74164 LUMO: 1.37690 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10475.54241 HOMO: -6.47359 LUMO: -0.59321 factor:1 | 1 (-2.80367) | -1 | -1 |
| G: -2104.18652 HOMO: -7.74164 LUMO: 1.37690 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10475.80070 HOMO: -6.52257 LUMO: -0.54695 factor:1 | 1 (-3.06196) | -1 | -1 |
| G: -2104.18652 HOMO: -7.74164 LUMO: 1.37690 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10475.43979 HOMO: -6.61781 LUMO: -0.69661 factor:1 | 1 (-2.70106) | -1 | -1 |
| G: -2104.18652 HOMO: -7.74164 LUMO: 1.37690 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10475.31201 HOMO: -6.77564 LUMO: -0.80001 factor:1 | 1 (-2.57327) | -1 | -1 |
| G: -2104.18652 HOMO: -7.74164 LUMO: 1.37690 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10475.60793 HOMO: -7.35252 LUMO: -1.00410 factor:1 | 1 (-2.86920) | -1 | -1 |
| G: -2104.18652 HOMO: -7.74164 LUMO: 1.37690 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10475.74467 HOMO: -6.35386 LUMO: -0.38912 factor:1 | 1 (-3.00593) | -1 | -1 |
| G: -2104.18652 HOMO: -7.74164 LUMO: 1.37690 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10475.64080 HOMO: -6.80285 LUMO: -0.52246 factor:1 | 1 (-2.90207) | -1 | -1 |
| G: -2104.18652 HOMO: -7.74164 LUMO: 1.37690 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10476.39151 HOMO: -7.23279 LUMO: 0.30477 factor:1 | 1 (-3.65277) | -1 | -1 |
| G: -2104.18652 HOMO: -7.74164 LUMO: 1.37690 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10475.82660 HOMO: -7.13483 LUMO: -0.76192 factor:1 | 1 (-3.08787) | -1 | -1 |
| G: -2104.18652 HOMO: -7.74164 LUMO: 1.37690 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10475.46483 HOMO: -6.71849 LUMO: -0.48164 factor:1 | 1 (-2.72609) | -1 | -1 |
| G: -2104.18652 HOMO: -7.74164 LUMO: 1.37690 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10475.29462 HOMO: -6.85455 LUMO: -0.69389 factor:1 | 1 (-2.55588) | -1 | -1 |
| G: -2104.18652 HOMO: -7.74164 LUMO: 1.37690 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10475.31244 HOMO: -6.96339 LUMO: -0.73743 factor:1 | 1 (-2.57371) | -1 | -1 |
| G: -2104.18652 HOMO: -7.74164 LUMO: 1.37690 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10475.99733 HOMO: -7.50490 LUMO: 0.28844 factor:1 | 1 (-3.25859) | -1 | -1 |
| G: -2104.18652 HOMO: -7.74164 LUMO: 1.37690 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10476.21638 HOMO: -6.63958 LUMO: -0.50069 factor:1 | 1 (-3.47764) | -1 | -1 |
| G: -2104.18652 HOMO: -7.74164 LUMO: 1.37690 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10476.04506 HOMO: -6.78924 LUMO: -0.69661 factor:1 | 1 (-3.30632) | -1 | -1 |
| G: -2104.18652 HOMO: -7.74164 LUMO: 1.37690 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10476.85190 HOMO: -7.44776 LUMO: 0.33742 factor:1 | 1 (-4.11316) | -1 | -1 |
| G: -2104.18652 HOMO: -7.74164 LUMO: 1.37690 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10475.30782 HOMO: -6.15249 LUMO: 0.66396 factor:1 | 1 (-2.56908) | -1 | -1 |
| G: -2104.18652 HOMO: -7.74164 LUMO: 1.37690 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10475.54377 HOMO: -6.17426 LUMO: 0.55511 factor:1 | 1 (-2.80503) | -1 | -1 |
| G: -2104.18652 HOMO: -7.74164 LUMO: 1.37690 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10475.71343 HOMO: -6.83550 LUMO: 0.28844 factor:1 | 1 (-2.97469) | -1 | -1 |
| G: -2104.18652 HOMO: -7.74164 LUMO: 1.37690 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10475.30183 HOMO: -6.32393 LUMO: 0.47620 factor:1 | 1 (-2.56309) | -1 | -1 |
| G: -2104.18652 HOMO: -7.74164 LUMO: 1.37690 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10475.52611 HOMO: -6.32937 LUMO: 0.45987 factor:1 | 1 (-2.78737) | -1 | -1 |
| G: -2104.18652 HOMO: -7.74164 LUMO: 1.37690 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10475.98620 HOMO: -7.37429 LUMO: 0.09252 factor:1 | 1 (-3.24746) | -1 | -1 |
| G: -2104.18652 HOMO: -7.74164 LUMO: 1.37690 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10475.41163 HOMO: -6.54434 LUMO: -0.39729 factor:1 | 1 (-2.67289) | -1 | -1 |
| G: -2104.18652 HOMO: -7.74164 LUMO: 1.37690 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10476.64387 HOMO: -7.35524 LUMO: 0.28028 factor:1 | 1 (-3.90513) | -1 | -1 |
| G: -2104.18652 HOMO: -7.74164 LUMO: 1.37690 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10475.77830 HOMO: -6.95523 LUMO: -0.86804 factor:1 | 1 (-3.03957) | -1 | -1 |
| G: -2104.18652 HOMO: -7.74164 LUMO: 1.37690 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10475.99499 HOMO: -6.63958 LUMO: -0.65307 factor:1 | 1 (-3.25625) | -1 | -1 |
| G: -2104.18652 HOMO: -7.74164 LUMO: 1.37690 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10476.00407 HOMO: -6.73482 LUMO: -0.67212 factor:1 | 1 (-3.26534) | -1 | -1 |
| G: -2104.18652 HOMO: -7.74164 LUMO: 1.37690 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10475.66853 HOMO: -6.37835 LUMO: -0.53606 factor:1 | 1 (-2.92980) | -1 | -1 |
| G: -2104.18652 HOMO: -7.74164 LUMO: 1.37690 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10475.81085 HOMO: -6.71849 LUMO: -0.61226 factor:1 | 1 (-3.07211) | -1 | -1 |
| G: -2104.18652 HOMO: -7.74164 LUMO: 1.37690 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10475.52744 HOMO: -6.68584 LUMO: -1.11022 factor:1 | 1 (-2.78870) | -1 | -1 |
| G: -2104.18652 HOMO: -7.74164 LUMO: 1.37690 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10475.52344 HOMO: -6.80285 LUMO: -0.79185 factor:1 | 1 (-2.78470) | -1 | -1 |
| G: -2104.18652 HOMO: -7.74164 LUMO: 1.37690 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10475.56445 HOMO: -7.14571 LUMO: -0.94696 factor:1 | 1 (-2.82571) | -1 | -1 |
| G: -2104.18652 HOMO: -7.74164 LUMO: 1.37690 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10475.94750 HOMO: -7.16204 LUMO: -0.66124 factor:1 | 1 (-3.20877) | -1 | -1 |
| G: -2104.18652 HOMO: -7.74164 LUMO: 1.37690 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10476.01874 HOMO: -6.54978 LUMO: -0.54967 factor:1 | 1 (-3.28001) | -1 | -1 |
| G: -2104.18652 HOMO: -7.74164 LUMO: 1.37690 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10475.81743 HOMO: -6.75114 LUMO: -0.70750 factor:1 | 1 (-3.07870) | -1 | -1 |
| G: -2104.18652 HOMO: -7.74164 LUMO: 1.37690 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10476.47102 HOMO: -7.22190 LUMO: 0.39184 factor:1 | 1 (-3.73229) | -1 | -1 |
| G: -2104.18652 HOMO: -7.74164 LUMO: 1.37690 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10475.96192 HOMO: -7.43959 LUMO: 0.30477 factor:1 | 1 (-3.22319) | -1 | -1 |
| G: -2104.18652 HOMO: -7.74164 LUMO: 1.37690 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10475.19260 HOMO: -6.87360 LUMO: -0.77552 factor:1 | 1 (-2.45387) | -1 | -1 |
| G: -2104.18652 HOMO: -7.74164 LUMO: 1.37690 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10475.53490 HOMO: -6.82734 LUMO: -0.59593 factor:1 | 1 (-2.79616) | -1 | -1 |
| G: -2104.18652 HOMO: -7.74164 LUMO: 1.37690 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10475.38961 HOMO: -6.65318 LUMO: -0.46259 factor:1 | 1 (-2.65088) | -1 | -1 |
| G: -2104.18652 HOMO: -7.74164 LUMO: 1.37690 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10475.46502 HOMO: -7.05863 LUMO: -1.17009 factor:1 | 1 (-2.72628) | -1 | -1 |
| G: -2104.18652 HOMO: -7.74164 LUMO: 1.37690 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10475.60001 HOMO: -6.57427 LUMO: -0.48708 factor:1 | 1 (-2.86128) | -1 | -1 |
| G: -2104.18652 HOMO: -7.74164 LUMO: 1.37690 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10475.80138 HOMO: -6.60420 LUMO: -0.38096 factor:1 | 1 (-3.06264) | -1 | -1 |
| G: -2104.18652 HOMO: -7.74164 LUMO: 1.37690 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10475.79833 HOMO: -6.72121 LUMO: -0.66668 factor:1 | 1 (-3.05959) | -1 | -1 |
| G: -2104.18652 HOMO: -7.74164 LUMO: 1.37690 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10475.55468 HOMO: -6.52257 LUMO: -0.19320 factor:1 | 1 (-2.81594) | -1 | -1 |
| G: -2104.18652 HOMO: -7.74164 LUMO: 1.37690 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10476.38669 HOMO: -6.28039 LUMO: -0.27211 factor:1 | 1 (-3.64796) | -1 | -1 |
| G: -2104.18652 HOMO: -7.74164 LUMO: 1.37690 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10476.39461 HOMO: -6.71849 LUMO: -0.42722 factor:1 | 1 (-3.65588) | -1 | -1 |
| G: -2104.18652 HOMO: -7.74164 LUMO: 1.37690 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10475.65596 HOMO: -6.27495 LUMO: 0.27756 factor:1 | 1 (-2.91722) | -1 | -1 |
| G: -2104.18652 HOMO: -7.74164 LUMO: 1.37690 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10475.68880 HOMO: -6.21780 LUMO: 0.46531 factor:1 | 1 (-2.95007) | -1 | -1 |
| G: -2104.18652 HOMO: -7.74164 LUMO: 1.37690 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10476.02658 HOMO: -6.52257 LUMO: -0.64491 factor:1 | 1 (-3.28784) | -1 | -1 |
| G: -2104.18652 HOMO: -7.74164 LUMO: 1.37690 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10474.56742 HOMO: -6.73754 LUMO: 1.83133 factor:1 | 1 (-1.82869) | -1 | -1 |
| G: -2104.18652 HOMO: -7.74164 LUMO: 1.37690 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10474.70680 HOMO: -6.67223 LUMO: 1.88847 factor:1 | 1 (-1.96806) | -1 | -1 |
| G: -2104.18652 HOMO: -7.74164 LUMO: 1.37690 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10474.48024 HOMO: -6.82189 LUMO: 1.59187 factor:1 | 1 (-1.74150) | -1 | -1 |
| G: -2104.18652 HOMO: -7.74164 LUMO: 1.37690 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10474.82318 HOMO: -6.43277 LUMO: 1.76330 factor:1 | 1 (-2.08445) | -1 | -1 |
| G: -2104.18652 HOMO: -7.74164 LUMO: 1.37690 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10474.54421 HOMO: -6.48175 LUMO: 1.77962 factor:1 | 1 (-1.80548) | -1 | -1 |
| G: -2104.18652 HOMO: -7.74164 LUMO: 1.37690 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10474.75134 HOMO: -6.50352 LUMO: 1.68438 factor:1 | 1 (-2.01261) | -1 | -1 |
| G: -2104.18652 HOMO: -7.74164 LUMO: 1.37690 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10474.05819 HOMO: -6.31576 LUMO: 2.03813 factor:1 | 1 (-1.31945) | -1 | -1 |
| G: -2104.18652 HOMO: -7.74164 LUMO: 1.37690 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10474.00461 HOMO: -6.27495 LUMO: 1.99459 factor:1 | 1 (-1.26587) | -1 | -1 |
| G: -2104.18652 HOMO: -7.74164 LUMO: 1.37690 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10473.94466 HOMO: -6.23957 LUMO: 2.17147 factor:1 | 1 (-1.20593) | -1 | -1 |
| G: -2104.18652 HOMO: -7.74164 LUMO: 1.37690 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10474.25661 HOMO: -6.78108 LUMO: 2.16875 factor:1 | 1 (-1.51788) | -1 | -1 |
| G: -2104.18652 HOMO: -7.74164 LUMO: 1.37690 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10474.27713 HOMO: -6.34297 LUMO: 2.10344 factor:1 | 1 (-1.53840) | -1 | -1 |
| G: -2104.18652 HOMO: -7.74164 LUMO: 1.37690 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10474.14883 HOMO: -6.30216 LUMO: 2.00004 factor:1 | 1 (-1.41009) | -1 | -1 |
| G: -2104.18652 HOMO: -7.74164 LUMO: 1.37690 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10474.51735 HOMO: -6.72665 LUMO: 2.09528 factor:1 | 1 (-1.77862) | -1 | -1 |
| G: -2104.18652 HOMO: -7.74164 LUMO: 1.37690 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10474.55757 HOMO: -6.86543 LUMO: 1.91568 factor:1 | 1 (-1.81884) | -1 | -1 |
| G: -2104.18652 HOMO: -7.74164 LUMO: 1.37690 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10474.15969 HOMO: -5.83956 LUMO: 1.89391 factor:1 | 1 (-1.42095) | -1 | -1 |
| G: -2104.18652 HOMO: -7.74164 LUMO: 1.37690 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10474.05011 HOMO: -6.42189 LUMO: 2.03269 factor:1 | 1 (-1.31137) | -1 | -1 |
| G: -2104.18652 HOMO: -7.74164 LUMO: 1.37690 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10474.44709 HOMO: -6.07630 LUMO: 1.80956 factor:1 | 1 (-1.70836) | -1 | -1 |
| G: -2104.18652 HOMO: -7.74164 LUMO: 1.37690 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10474.29123 HOMO: -6.43277 LUMO: 1.81772 factor:1 | 1 (-1.55249) | -1 | -1 |
| G: -2104.18652 HOMO: -7.74164 LUMO: 1.37690 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10474.70307 HOMO: -7.03959 LUMO: 1.78779 factor:1 | 1 (-1.96434) | -1 | -1 |
| G: -2104.18652 HOMO: -7.74164 LUMO: 1.37690 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10475.34959 HOMO: -6.72121 LUMO: 2.29664 factor:1 | 1 (-2.61085) | -1 | -1 |
| G: -2104.18652 HOMO: -7.74164 LUMO: 1.37690 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10475.24741 HOMO: -6.62869 LUMO: 2.04630 factor:1 | 1 (-2.50867) | -1 | -1 |
| G: -2104.18652 HOMO: -7.74164 LUMO: 1.37690 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10475.21889 HOMO: -6.63958 LUMO: 1.84221 factor:1 | 1 (-2.48015) | -1 | -1 |
| G: -2104.18652 HOMO: -7.74164 LUMO: 1.37690 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10475.01317 HOMO: -6.70761 LUMO: 1.67350 factor:1 | 1 (-2.27444) | -1 | -1 |
| G: -2104.18652 HOMO: -7.74164 LUMO: 1.37690 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10474.50326 HOMO: -6.00283 LUMO: 1.64357 factor:1 | 1 (-1.76452) | -1 | -1 |
| G: -2104.18652 HOMO: -7.74164 LUMO: 1.37690 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10474.38407 HOMO: -6.48719 LUMO: 1.70343 factor:1 | 1 (-1.64534) | -1 | -1 |
| G: -2104.18652 HOMO: -7.74164 LUMO: 1.37690 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10474.51273 HOMO: -6.13345 LUMO: 1.44492 factor:1 | 1 (-1.77399) | -1 | -1 |
| G: -2104.18652 HOMO: -7.74164 LUMO: 1.37690 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10474.58024 HOMO: -6.11168 LUMO: 1.70071 factor:1 | 1 (-1.84150) | -1 | -1 |
| G: -2104.18652 HOMO: -7.74164 LUMO: 1.37690 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10474.52554 HOMO: -6.09535 LUMO: 1.82316 factor:1 | 1 (-1.78681) | -1 | -1 |
| G: -2104.18652 HOMO: -7.74164 LUMO: 1.37690 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10474.88833 HOMO: -6.81101 LUMO: 1.63540 factor:1 | 1 (-2.14959) | -1 | -1 |
| G: -2104.18652 HOMO: -7.74164 LUMO: 1.37690 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10474.77896 HOMO: -6.80013 LUMO: 2.12249 factor:1 | 1 (-2.04023) | -1 | -1 |
| G: -2104.18652 HOMO: -7.74164 LUMO: 1.37690 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10474.54035 HOMO: -6.48447 LUMO: 1.94561 factor:1 | 1 (-1.80161) | -1 | -1 |
| G: -2104.18652 HOMO: -7.74164 LUMO: 1.37690 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10474.67025 HOMO: -6.72393 LUMO: 2.06534 factor:1 | 1 (-1.93152) | -1 | -1 |
| G: -2104.18652 HOMO: -7.74164 LUMO: 1.37690 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10474.39387 HOMO: -6.34570 LUMO: 1.98915 factor:1 | 1 (-1.65513) | -1 | -1 |
| G: -2104.18652 HOMO: -7.74164 LUMO: 1.37690 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10474.27825 HOMO: -6.31304 LUMO: 1.87759 factor:1 | 1 (-1.53951) | -1 | -1 |
| G: -2104.18652 HOMO: -7.74164 LUMO: 1.37690 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10474.62136 HOMO: -6.77564 LUMO: 1.81228 factor:1 | 1 (-1.88262) | -1 | -1 |
| G: -2104.18652 HOMO: -7.74164 LUMO: 1.37690 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10475.19380 HOMO: -6.58516 LUMO: 2.34834 factor:1 | 1 (-2.45507) | -1 | -1 |
| G: -2104.18652 HOMO: -7.74164 LUMO: 1.37690 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10475.32398 HOMO: -6.68040 LUMO: 2.20412 factor:1 | 1 (-2.58524) | -1 | -1 |
| G: -2104.18652 HOMO: -7.74164 LUMO: 1.37690 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10475.21867 HOMO: -6.20964 LUMO: 2.17147 factor:1 | 1 (-2.47994) | -1 | -1 |
| G: -2104.18652 HOMO: -7.74164 LUMO: 1.37690 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10475.14000 HOMO: -6.54706 LUMO: 2.03813 factor:1 | 1 (-2.40127) | -1 | -1 |
| G: -2104.18652 HOMO: -7.74164 LUMO: 1.37690 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10475.03173 HOMO: -6.54162 LUMO: 2.17419 factor:1 | 1 (-2.29299) | -1 | -1 |
| G: -2104.18652 HOMO: -7.74164 LUMO: 1.37690 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10475.09965 HOMO: -6.75659 LUMO: 2.22589 factor:1 | 1 (-2.36091) | -1 | -1 |
| G: -2104.18652 HOMO: -7.74164 LUMO: 1.37690 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10475.08381 HOMO: -6.59604 LUMO: 2.59325 factor:1 | 1 (-2.34508) | -1 | -1 |
| G: -2104.18652 HOMO: -7.74164 LUMO: 1.37690 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10475.17454 HOMO: -6.11712 LUMO: 2.02181 factor:1 | 1 (-2.43580) | -1 | -1 |
| G: -2104.18652 HOMO: -7.74164 LUMO: 1.37690 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10475.27843 HOMO: -6.63141 LUMO: 2.09256 factor:1 | 1 (-2.53969) | -1 | -1 |
| G: -2104.18652 HOMO: -7.74164 LUMO: 1.37690 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10474.74021 HOMO: -6.61781 LUMO: 1.86126 factor:1 | 1 (-2.00148) | -1 | -1 |
| G: -2104.18652 HOMO: -7.74164 LUMO: 1.37690 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10474.76574 HOMO: -6.63958 LUMO: 1.77146 factor:1 | 1 (-2.02700) | -1 | -1 |
| G: -2104.18652 HOMO: -7.74164 LUMO: 1.37690 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10474.64166 HOMO: -6.60420 LUMO: 1.54561 factor:1 | 1 (-1.90292) | -1 | -1 |
| G: -2104.18652 HOMO: -7.74164 LUMO: 1.37690 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10474.86773 HOMO: -6.52529 LUMO: 2.05174 factor:1 | 1 (-2.12899) | -1 | -1 |
| G: -2104.18652 HOMO: -7.74164 LUMO: 1.37690 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10475.10727 HOMO: -6.80285 LUMO: 2.13609 factor:1 | 1 (-2.36853) | -1 | -1 |
| G: -2104.18652 HOMO: -7.74164 LUMO: 1.37690 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10475.22352 HOMO: -6.51168 LUMO: 2.25855 factor:1 | 1 (-2.48478) | -1 | -1 |
| G: -2104.18652 HOMO: -7.74164 LUMO: 1.37690 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10475.27138 HOMO: -6.64774 LUMO: 2.46263 factor:1 | 1 (-2.53265) | -1 | -1 |
| G: -2104.18652 HOMO: -7.74164 LUMO: 1.37690 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10475.26442 HOMO: -6.40828 LUMO: 1.99732 factor:1 | 1 (-2.52568) | -1 | -1 |
| G: -2104.18652 HOMO: -7.74164 LUMO: 1.37690 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10475.41756 HOMO: -5.97562 LUMO: 1.56465 factor:1 | 1 (-2.67882) | -1 | -1 |
| G: -2104.18652 HOMO: -7.74164 LUMO: 1.37690 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10475.38104 HOMO: -6.75659 LUMO: 2.23405 factor:1 | 1 (-2.64231) | -1 | -1 |
| G: -2104.18652 HOMO: -7.74164 LUMO: 1.37690 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10475.53549 HOMO: -6.68584 LUMO: 2.09528 factor:1 | 1 (-2.79676) | -1 | -1 |
| G: -2104.18652 HOMO: -7.74164 LUMO: 1.37690 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10475.48232 HOMO: -6.86543 LUMO: 1.95106 factor:1 | 1 (-2.74359) | -1 | -1 |
| G: -2104.18652 HOMO: -7.74164 LUMO: 1.37690 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10473.40993 HOMO: -6.47359 LUMO: 1.82316 factor:1 | 1 (-0.67120) | -1 | -1 |
| G: -2104.18652 HOMO: -7.74164 LUMO: 1.37690 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10473.77620 HOMO: -6.87632 LUMO: 2.08439 factor:1 | 1 (-1.03746) | -1 | -1 |
| G: -2104.18652 HOMO: -7.74164 LUMO: 1.37690 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10473.38650 HOMO: -6.33753 LUMO: 2.16603 factor:1 | 1 (-0.64777) | -1 | -1 |
| G: -2104.18652 HOMO: -7.74164 LUMO: 1.37690 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10473.86368 HOMO: -6.92258 LUMO: 1.72248 factor:1 | 1 (-1.12495) | -1 | -1 |
| G: -2104.18652 HOMO: -7.74164 LUMO: 1.37690 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10474.55907 HOMO: -6.62597 LUMO: 2.10344 factor:1 | 1 (-1.82033) | -1 | -1 |
| G: -2104.18652 HOMO: -7.74164 LUMO: 1.37690 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10474.45665 HOMO: -6.63141 LUMO: 1.94017 factor:1 | 1 (-1.71791) | -1 | -1 |
| G: -2104.18652 HOMO: -7.74164 LUMO: 1.37690 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10474.52941 HOMO: -6.48447 LUMO: 1.91840 factor:1 | 1 (-1.79067) | -1 | -1 |
| G: -2104.18652 HOMO: -7.74164 LUMO: 1.37690 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10474.38859 HOMO: -6.41372 LUMO: 1.61364 factor:1 | 1 (-1.64985) | -1 | -1 |
| G: -2104.18652 HOMO: -7.74164 LUMO: 1.37690 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10474.14842 HOMO: -6.37291 LUMO: 1.79051 factor:1 | 1 (-1.40969) | -1 | -1 |
| G: -2104.18652 HOMO: -7.74164 LUMO: 1.37690 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10474.21079 HOMO: -6.13073 LUMO: 1.77962 factor:1 | 1 (-1.47205) | -1 | -1 |
| G: -2104.18652 HOMO: -7.74164 LUMO: 1.37690 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10474.01348 HOMO: -6.13073 LUMO: 1.98915 factor:1 | 1 (-1.27474) | -1 | -1 |
| G: -2104.18652 HOMO: -7.74164 LUMO: 1.37690 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10474.43776 HOMO: -6.44094 LUMO: 1.58370 factor:1 | 1 (-1.69902) | -1 | -1 |
| G: -2104.18652 HOMO: -7.74164 LUMO: 1.37690 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10476.35728 HOMO: -6.87087 LUMO: -0.82995 factor:1 | 1 (-3.61854) | -1 | -1 |
| G: -2104.18652 HOMO: -7.74164 LUMO: 1.37690 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10474.40421 HOMO: -6.67223 LUMO: 1.08029 factor:1 | 1 (-1.66547) | -1 | -1 |
| G: -2104.18652 HOMO: -7.74164 LUMO: 1.37690 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10474.01903 HOMO: -6.82462 LUMO: 0.91702 factor:1 | 1 (-1.28030) | -1 | -1 |
| G: -2104.18652 HOMO: -7.74164 LUMO: 1.37690 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10474.77782 HOMO: -6.65863 LUMO: 1.52656 factor:1 | 1 (-2.03909) | -1 | -1 |
| G: -2104.18652 HOMO: -7.74164 LUMO: 1.37690 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10474.36494 HOMO: -6.78924 LUMO: 0.86260 factor:1 | 1 (-1.62621) | -1 | -1 |
| G: -2104.18652 HOMO: -7.74164 LUMO: 1.37690 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10474.39849 HOMO: -6.68584 LUMO: 0.94424 factor:1 | 1 (-1.65976) | -1 | -1 |
| G: -2104.18652 HOMO: -7.74164 LUMO: 1.37690 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10474.57583 HOMO: -6.58788 LUMO: 1.00138 factor:1 | 1 (-1.83710) | -1 | -1 |
| G: -2104.18652 HOMO: -7.74164 LUMO: 1.37690 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10474.62304 HOMO: -6.79740 LUMO: 0.91430 factor:1 | 1 (-1.88431) | -1 | -1 |
| G: -2104.18652 HOMO: -7.74164 LUMO: 1.37690 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10473.94401 HOMO: -6.67223 LUMO: 0.80274 factor:1 | 1 (-1.20527) | -1 | -1 |
| G: -2104.18652 HOMO: -7.74164 LUMO: 1.37690 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10474.14287 HOMO: -6.95251 LUMO: 0.90614 factor:1 | 1 (-1.40413) | -1 | -1 |
| G: -2104.18652 HOMO: -7.74164 LUMO: 1.37690 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10474.40897 HOMO: -7.19469 LUMO: 1.34152 factor:1 | 1 (-1.67023) | -1 | -1 |
| G: -2104.18652 HOMO: -7.74164 LUMO: 1.37690 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10475.31220 HOMO: -6.59332 LUMO: -0.76464 factor:1 | 1 (-2.57346) | -1 | -1 |
| G: -2104.18652 HOMO: -7.74164 LUMO: 1.37690 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10475.44529 HOMO: -6.77564 LUMO: -0.90886 factor:1 | 1 (-2.70655) | -1 | -1 |
| G: -2104.18652 HOMO: -7.74164 LUMO: 1.37690 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10475.27203 HOMO: -6.57971 LUMO: -0.41633 factor:1 | 1 (-2.53330) | -1 | -1 |
| G: -2104.18652 HOMO: -7.74164 LUMO: 1.37690 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10475.38469 HOMO: -6.68856 LUMO: -0.58232 factor:1 | 1 (-2.64595) | -1 | -1 |
| G: -2104.18652 HOMO: -7.74164 LUMO: 1.37690 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10476.21143 HOMO: -6.87087 LUMO: -0.71022 factor:1 | 1 (-3.47269) | -1 | -1 |
| G: -2104.18652 HOMO: -7.74164 LUMO: 1.37690 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10476.12130 HOMO: -6.67767 LUMO: -0.74559 factor:1 | 1 (-3.38257) | -1 | -1 |
| G: -2104.18652 HOMO: -7.74164 LUMO: 1.37690 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10476.14889 HOMO: -6.68040 LUMO: -0.65307 factor:1 | 1 (-3.41016) | -1 | -1 |
| G: -2104.18652 HOMO: -7.74164 LUMO: 1.37690 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10475.57079 HOMO: -6.32937 LUMO: 0.80274 factor:1 | 1 (-2.83205) | -1 | -1 |
| G: -2104.18652 HOMO: -7.74164 LUMO: 1.37690 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10475.60222 HOMO: -6.29671 LUMO: 0.82723 factor:1 | 1 (-2.86348) | -1 | -1 |
| G: -2104.18652 HOMO: -7.74164 LUMO: 1.37690 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10475.64020 HOMO: -6.67767 LUMO: 0.59321 factor:1 | 1 (-2.90147) | -1 | -1 |
| G: -2104.18652 HOMO: -7.74164 LUMO: 1.37690 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10475.69201 HOMO: -6.77836 LUMO: 0.50341 factor:1 | 1 (-2.95328) | -1 | -1 |
| G: -2104.18652 HOMO: -7.74164 LUMO: 1.37690 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10475.26969 HOMO: -6.61781 LUMO: 0.42450 factor:1 | 1 (-2.53096) | -1 | -1 |
| G: -2104.18652 HOMO: -7.74164 LUMO: 1.37690 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10475.65748 HOMO: -6.83278 LUMO: 0.39457 factor:1 | 1 (-2.91875) | -1 | -1 |
| G: -2104.18652 HOMO: -7.74164 LUMO: 1.37690 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10475.47928 HOMO: -6.56883 LUMO: 0.64219 factor:1 | 1 (-2.74054) | -1 | -1 |
| G: -2104.18652 HOMO: -7.74164 LUMO: 1.37690 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10475.67982 HOMO: -6.71577 LUMO: 0.40001 factor:1 | 1 (-2.94109) | -1 | -1 |
| G: -2104.18652 HOMO: -7.74164 LUMO: 1.37690 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10475.30461 HOMO: -6.86543 LUMO: -0.74287 factor:1 | 1 (-2.56587) | -1 | -1 |
| G: -2104.18652 HOMO: -7.74164 LUMO: 1.37690 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10475.10294 HOMO: -6.68584 LUMO: -0.69389 factor:1 | 1 (-2.36421) | -1 | -1 |
| G: -2104.18652 HOMO: -7.74164 LUMO: 1.37690 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10475.32918 HOMO: -6.61237 LUMO: -0.48980 factor:1 | 1 (-2.59044) | -1 | -1 |
| G: -2104.18652 HOMO: -7.74164 LUMO: 1.37690 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10475.37117 HOMO: -6.80285 LUMO: -0.58232 factor:1 | 1 (-2.63243) | -1 | -1 |
| G: -2104.18652 HOMO: -7.74164 LUMO: 1.37690 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10475.18243 HOMO: -6.88992 LUMO: -0.70205 factor:1 | 1 (-2.44369) | -1 | -1 |
| G: -2104.18652 HOMO: -7.74164 LUMO: 1.37690 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10475.15606 HOMO: -6.95251 LUMO: -0.71838 factor:1 | 1 (-2.41732) | -1 | -1 |
| G: -2104.18652 HOMO: -7.74164 LUMO: 1.37690 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10475.94805 HOMO: -7.52123 LUMO: 0.27211 factor:1 | 1 (-3.20931) | -1 | -1 |
| G: -2104.18652 HOMO: -7.74164 LUMO: 1.37690 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10475.41098 HOMO: -6.76747 LUMO: -0.74015 factor:1 | 1 (-2.67224) | -1 | -1 |
| G: -2104.18652 HOMO: -7.74164 LUMO: 1.37690 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10475.51544 HOMO: -6.55250 LUMO: -0.49797 factor:1 | 1 (-2.77670) | -1 | -1 |
| G: -2104.18652 HOMO: -7.74164 LUMO: 1.37690 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10475.27579 HOMO: -6.50896 LUMO: -0.46804 factor:1 | 1 (-2.53705) | -1 | -1 |
| G: -2104.18652 HOMO: -7.74164 LUMO: 1.37690 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10475.96320 HOMO: -7.45320 LUMO: 0.08436 factor:1 | 1 (-3.22447) | -1 | -1 |
| G: -2104.18652 HOMO: -7.74164 LUMO: 1.37690 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10475.50145 HOMO: -6.82462 LUMO: -0.70477 factor:1 | 1 (-2.76272) | -1 | -1 |
| G: -2104.18652 HOMO: -7.74164 LUMO: 1.37690 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10475.15728 HOMO: -6.57155 LUMO: -0.43538 factor:1 | 1 (-2.41855) | -1 | -1 |
| G: -2104.18652 HOMO: -7.74164 LUMO: 1.37690 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10475.29051 HOMO: -6.72665 LUMO: -0.55239 factor:1 | 1 (-2.55177) | -1 | -1 |
| G: -2104.18652 HOMO: -7.74164 LUMO: 1.37690 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10475.48850 HOMO: -7.05319 LUMO: -1.08573 factor:1 | 1 (-2.74976) | -1 | -1 |
| G: -2104.18652 HOMO: -7.74164 LUMO: 1.37690 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10475.42627 HOMO: -6.56067 LUMO: -0.45715 factor:1 | 1 (-2.68753) | -1 | -1 |
| G: -2104.18652 HOMO: -7.74164 LUMO: 1.37690 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10475.22939 HOMO: -6.76475 LUMO: -0.53879 factor:1 | 1 (-2.49066) | -1 | -1 |
| G: -2104.18652 HOMO: -7.74164 LUMO: 1.37690 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10475.44377 HOMO: -6.67223 LUMO: -0.45987 factor:1 | 1 (-2.70503) | -1 | -1 |
| G: -2104.18652 HOMO: -7.74164 LUMO: 1.37690 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10476.03866 HOMO: -6.44094 LUMO: -0.72110 factor:1 | 1 (-3.29992) | -1 | -1 |
| G: -2104.18652 HOMO: -7.74164 LUMO: 1.37690 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10476.02571 HOMO: -6.66951 LUMO: -0.67756 factor:1 | 1 (-3.28697) | -1 | -1 |
| G: -2104.18652 HOMO: -7.74164 LUMO: 1.37690 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10476.17812 HOMO: -6.69400 LUMO: -0.62858 factor:1 | 1 (-3.43938) | -1 | -1 |
| G: -2104.18652 HOMO: -7.74164 LUMO: 1.37690 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10476.25151 HOMO: -6.51985 LUMO: -0.37007 factor:1 | 1 (-3.51277) | -1 | -1 |
| G: -2104.18652 HOMO: -7.74164 LUMO: 1.37690 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10475.69346 HOMO: -5.98378 LUMO: 0.78641 factor:1 | 1 (-2.95472) | -1 | -1 |
| G: -2104.18652 HOMO: -7.74164 LUMO: 1.37690 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10475.65961 HOMO: -6.11440 LUMO: 0.71294 factor:1 | 1 (-2.92087) | -1 | -1 |
| G: -2104.18652 HOMO: -7.74164 LUMO: 1.37690 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10475.78736 HOMO: -6.45182 LUMO: 0.63947 factor:1 | 1 (-3.04863) | -1 | -1 |
| G: -2104.18652 HOMO: -7.74164 LUMO: 1.37690 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10475.53560 HOMO: -6.78924 LUMO: 0.37007 factor:1 | 1 (-2.79687) | -1 | -1 |
| G: -2104.18652 HOMO: -7.74164 LUMO: 1.37690 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10475.63585 HOMO: -6.63686 LUMO: 0.54423 factor:1 | 1 (-2.89711) | -1 | -1 |
| G: -2104.18652 HOMO: -7.74164 LUMO: 1.37690 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10475.52665 HOMO: -6.66679 LUMO: 0.48708 factor:1 | 1 (-2.78792) | -1 | -1 |
| G: -2104.18652 HOMO: -7.74164 LUMO: 1.37690 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10475.64818 HOMO: -6.81917 LUMO: 0.31021 factor:1 | 1 (-2.90944) | -1 | -1 |
| G: -2104.18652 HOMO: -7.74164 LUMO: 1.37690 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10475.79509 HOMO: -6.28583 LUMO: 0.44899 factor:1 | 1 (-3.05636) | -1 | -1 |
| G: -2104.18652 HOMO: -7.74164 LUMO: 1.37690 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10475.80954 HOMO: -6.61237 LUMO: 0.49525 factor:1 | 1 (-3.07080) | -1 | -1 |
| G: -2104.18652 HOMO: -7.74164 LUMO: 1.37690 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10477.20957 HOMO: -7.08857 LUMO: 0.38368 factor:1 | 1 (-4.47083) | -1 | -1 |
| G: -2104.18652 HOMO: -7.74164 LUMO: 1.37690 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10476.34408 HOMO: -6.53890 LUMO: -0.68845 factor:1 | 1 (-3.60535) | -1 | -1 |
| G: -2104.18652 HOMO: -7.74164 LUMO: 1.37690 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10476.46474 HOMO: -6.56611 LUMO: -0.66396 factor:1 | 1 (-3.72600) | -1 | -1 |
| G: -2104.18652 HOMO: -7.74164 LUMO: 1.37690 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10476.25831 HOMO: -6.04909 LUMO: -0.59865 factor:1 | 1 (-3.51958) | -1 | -1 |
| G: -2104.18652 HOMO: -7.74164 LUMO: 1.37690 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10476.63894 HOMO: -6.74842 LUMO: -0.77825 factor:1 | 1 (-3.90021) | -1 | -1 |
| G: -2104.18652 HOMO: -7.74164 LUMO: 1.37690 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10475.39054 HOMO: -6.82462 LUMO: -0.61498 factor:1 | 1 (-2.65180) | -1 | -1 |
| G: -2104.18652 HOMO: -7.74164 LUMO: 1.37690 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10476.09161 HOMO: -7.40694 LUMO: 0.32926 factor:1 | 1 (-3.35288) | -1 | -1 |
| G: -2104.18652 HOMO: -7.74164 LUMO: 1.37690 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10475.44923 HOMO: -6.80557 LUMO: -0.57416 factor:1 | 1 (-2.71050) | -1 | -1 |
| G: -2104.18652 HOMO: -7.74164 LUMO: 1.37690 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10475.66709 HOMO: -6.76747 LUMO: -0.67484 factor:1 | 1 (-2.92835) | -1 | -1 |
| G: -2104.18652 HOMO: -7.74164 LUMO: 1.37690 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10476.56430 HOMO: -7.23279 LUMO: 0.48980 factor:1 | 1 (-3.82557) | -1 | -1 |
| G: -2104.18652 HOMO: -7.74164 LUMO: 1.37690 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10475.42317 HOMO: -6.62869 LUMO: -0.24762 factor:1 | 1 (-2.68443) | -1 | -1 |
| G: -2104.18652 HOMO: -7.74164 LUMO: 1.37690 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10475.80573 HOMO: -6.65863 LUMO: -0.28028 factor:1 | 1 (-3.06700) | -1 | -1 |
| G: -2104.18652 HOMO: -7.74164 LUMO: 1.37690 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10475.53824 HOMO: -6.50352 LUMO: -0.44899 factor:1 | 1 (-2.79951) | -1 | -1 |
| G: -2104.18652 HOMO: -7.74164 LUMO: 1.37690 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10475.58548 HOMO: -6.62053 LUMO: -0.88437 factor:1 | 1 (-2.84675) | -1 | -1 |
| G: -2104.18652 HOMO: -7.74164 LUMO: 1.37690 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10475.85466 HOMO: -6.73754 LUMO: -0.77825 factor:1 | 1 (-3.11592) | -1 | -1 |
| G: -2104.18652 HOMO: -7.74164 LUMO: 1.37690 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10476.78461 HOMO: -7.24639 LUMO: 0.35647 factor:1 | 1 (-4.04587) | -1 | -1 |
| G: -2104.18652 HOMO: -7.74164 LUMO: 1.37690 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10475.90097 HOMO: -6.46270 LUMO: -0.48164 factor:1 | 1 (-3.16224) | -1 | -1 |
| G: -2104.18652 HOMO: -7.74164 LUMO: 1.37690 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10475.59503 HOMO: -6.14161 LUMO: -0.66396 factor:1 | 1 (-2.85630) | -1 | -1 |
| G: -2104.18652 HOMO: -7.74164 LUMO: 1.37690 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10474.54808 HOMO: -6.63414 LUMO: 1.51295 factor:1 | 1 (-1.80934) | -1 | -1 |
| G: -2104.18652 HOMO: -7.74164 LUMO: 1.37690 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10474.30668 HOMO: -6.52529 LUMO: 1.65989 factor:1 | 1 (-1.56795) | -1 | -1 |
| G: -2104.18652 HOMO: -7.74164 LUMO: 1.37690 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10474.59733 HOMO: -6.63686 LUMO: 1.64629 factor:1 | 1 (-1.85859) | -1 | -1 |
| G: -2104.18652 HOMO: -7.74164 LUMO: 1.37690 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10474.44625 HOMO: -6.49808 LUMO: 1.60003 factor:1 | 1 (-1.70751) | -1 | -1 |
| G: -2104.18652 HOMO: -7.74164 LUMO: 1.37690 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10474.54900 HOMO: -6.85183 LUMO: 1.96194 factor:1 | 1 (-1.81026) | -1 | -1 |
| G: -2104.18652 HOMO: -7.74164 LUMO: 1.37690 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10474.42497 HOMO: -6.90081 LUMO: 1.82316 factor:1 | 1 (-1.68624) | -1 | -1 |
| G: -2104.18652 HOMO: -7.74164 LUMO: 1.37690 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10474.24981 HOMO: -6.20147 LUMO: 1.95106 factor:1 | 1 (-1.51108) | -1 | -1 |
| G: -2104.18652 HOMO: -7.74164 LUMO: 1.37690 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10474.53844 HOMO: -7.05047 LUMO: 1.94289 factor:1 | 1 (-1.79971) | -1 | -1 |
| G: -2104.18652 HOMO: -7.74164 LUMO: 1.37690 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10474.41229 HOMO: -6.11440 LUMO: 1.83949 factor:1 | 1 (-1.67355) | -1 | -1 |
| G: -2104.18652 HOMO: -7.74164 LUMO: 1.37690 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10474.47069 HOMO: -6.65046 LUMO: 1.59187 factor:1 | 1 (-1.73195) | -1 | -1 |
| G: -2104.18652 HOMO: -7.74164 LUMO: 1.37690 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10475.27982 HOMO: -6.81917 LUMO: 2.41365 factor:1 | 1 (-2.54108) | -1 | -1 |
| G: -2104.18652 HOMO: -7.74164 LUMO: 1.37690 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10475.05701 HOMO: -6.40284 LUMO: 2.48984 factor:1 | 1 (-2.31827) | -1 | -1 |
| G: -2104.18652 HOMO: -7.74164 LUMO: 1.37690 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10475.18194 HOMO: -7.04775 LUMO: 2.31025 factor:1 | 1 (-2.44320) | -1 | -1 |
| G: -2104.18652 HOMO: -7.74164 LUMO: 1.37690 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10475.24635 HOMO: -6.64774 LUMO: 2.20140 factor:1 | 1 (-2.50761) | -1 | -1 |
| G: -2104.18652 HOMO: -7.74164 LUMO: 1.37690 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10475.30763 HOMO: -6.72393 LUMO: 2.28304 factor:1 | 1 (-2.56889) | -1 | -1 |
| G: -2104.18652 HOMO: -7.74164 LUMO: 1.37690 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10474.30434 HOMO: -6.35114 LUMO: 1.84765 factor:1 | 1 (-1.56561) | -1 | -1 |
| G: -2104.18652 HOMO: -7.74164 LUMO: 1.37690 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10474.24268 HOMO: -6.41100 LUMO: 1.74697 factor:1 | 1 (-1.50395) | -1 | -1 |
| G: -2104.18652 HOMO: -7.74164 LUMO: 1.37690 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10474.32195 HOMO: -6.34297 LUMO: 1.55921 factor:1 | 1 (-1.58321) | -1 | -1 |
| G: -2104.18652 HOMO: -7.74164 LUMO: 1.37690 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10474.44952 HOMO: -6.31848 LUMO: 1.67622 factor:1 | 1 (-1.71078) | -1 | -1 |
| G: -2104.18652 HOMO: -7.74164 LUMO: 1.37690 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10474.30355 HOMO: -6.50896 LUMO: 2.02725 factor:1 | 1 (-1.56482) | -1 | -1 |
| G: -2104.18652 HOMO: -7.74164 LUMO: 1.37690 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10473.98915 HOMO: -6.28583 LUMO: 2.00548 factor:1 | 1 (-1.25042) | -1 | -1 |
| G: -2104.18652 HOMO: -7.74164 LUMO: 1.37690 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10474.51779 HOMO: -6.67495 LUMO: 1.92384 factor:1 | 1 (-1.77905) | -1 | -1 |
| G: -2104.18652 HOMO: -7.74164 LUMO: 1.37690 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10475.09984 HOMO: -6.17154 LUMO: 2.39732 factor:1 | 1 (-2.36110) | -1 | -1 |
| G: -2104.18652 HOMO: -7.74164 LUMO: 1.37690 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10475.34561 HOMO: -6.84911 LUMO: 2.24766 factor:1 | 1 (-2.60688) | -1 | -1 |
| G: -2104.18652 HOMO: -7.74164 LUMO: 1.37690 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10474.94925 HOMO: -6.77564 LUMO: 2.38372 factor:1 | 1 (-2.21052) | -1 | -1 |
| G: -2104.18652 HOMO: -7.74164 LUMO: 1.37690 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10474.84552 HOMO: -6.18243 LUMO: 2.40821 factor:1 | 1 (-2.10679) | -1 | -1 |
| G: -2104.18652 HOMO: -7.74164 LUMO: 1.37690 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10475.20855 HOMO: -6.40828 LUMO: 2.22589 factor:1 | 1 (-2.46981) | -1 | -1 |
| G: -2104.18652 HOMO: -7.74164 LUMO: 1.37690 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10475.18890 HOMO: -6.74570 LUMO: 1.88303 factor:1 | 1 (-2.45017) | -1 | -1 |
| G: -2104.18652 HOMO: -7.74164 LUMO: 1.37690 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10475.10302 HOMO: -6.29944 LUMO: 2.05174 factor:1 | 1 (-2.36429) | -1 | -1 |
| G: -2104.18652 HOMO: -7.74164 LUMO: 1.37690 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10475.55539 HOMO: -7.00693 LUMO: 2.16331 factor:1 | 1 (-2.81665) | -1 | -1 |
| G: -2104.18652 HOMO: -7.74164 LUMO: 1.37690 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10475.15856 HOMO: -6.89537 LUMO: 2.19596 factor:1 | 1 (-2.41983) | -1 | -1 |
| G: -2104.18652 HOMO: -7.74164 LUMO: 1.37690 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10475.24300 HOMO: -6.72665 LUMO: 2.03813 factor:1 | 1 (-2.50426) | -1 | -1 |
| G: -2104.18652 HOMO: -7.74164 LUMO: 1.37690 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10475.26077 HOMO: -6.69944 LUMO: 2.36467 factor:1 | 1 (-2.52203) | -1 | -1 |
| G: -2104.18652 HOMO: -7.74164 LUMO: 1.37690 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10475.35478 HOMO: -6.92802 LUMO: 1.72792 factor:1 | 1 (-2.61605) | -1 | -1 |
| G: -2104.18652 HOMO: -7.74164 LUMO: 1.37690 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10475.21440 HOMO: -6.12256 LUMO: 1.85310 factor:1 | 1 (-2.47566) | -1 | -1 |
| G: -2104.18652 HOMO: -7.74164 LUMO: 1.37690 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10475.18278 HOMO: -6.70489 LUMO: 2.20956 factor:1 | 1 (-2.44405) | -1 | -1 |
| G: -2104.18652 HOMO: -7.74164 LUMO: 1.37690 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10474.61523 HOMO: -6.94707 LUMO: 1.81500 factor:1 | 1 (-1.87650) | -1 | -1 |
| G: -2104.18652 HOMO: -7.74164 LUMO: 1.37690 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10474.37977 HOMO: -6.39468 LUMO: 1.79051 factor:1 | 1 (-1.64104) | -1 | -1 |
| G: -2104.18652 HOMO: -7.74164 LUMO: 1.37690 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10474.78133 HOMO: -6.69128 LUMO: 2.03813 factor:1 | 1 (-2.04260) | -1 | -1 |
| G: -2104.18652 HOMO: -7.74164 LUMO: 1.37690 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10474.36769 HOMO: -6.55250 LUMO: 2.00548 factor:1 | 1 (-1.62896) | -1 | -1 |
| G: -2104.18652 HOMO: -7.74164 LUMO: 1.37690 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10474.11190 HOMO: -6.24773 LUMO: 2.09256 factor:1 | 1 (-1.37317) | -1 | -1 |
| G: -2104.18652 HOMO: -7.74164 LUMO: 1.37690 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10474.61902 HOMO: -6.85727 LUMO: 1.70071 factor:1 | 1 (-1.88028) | -1 | -1 |
| G: -2104.18652 HOMO: -7.74164 LUMO: 1.37690 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10474.73913 HOMO: -6.71305 LUMO: 1.72520 factor:1 | 1 (-2.00039) | -1 | -1 |
| G: -2104.18652 HOMO: -7.74164 LUMO: 1.37690 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10474.76577 HOMO: -6.81101 LUMO: 2.15514 factor:1 | 1 (-2.02703) | -1 | -1 |
| G: -2104.18652 HOMO: -7.74164 LUMO: 1.37690 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10474.75719 HOMO: -6.93618 LUMO: 1.75513 factor:1 | 1 (-2.01846) | -1 | -1 |
| G: -2104.18652 HOMO: -7.74164 LUMO: 1.37690 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10475.02855 HOMO: -6.63686 LUMO: 2.09800 factor:1 | 1 (-2.28981) | -1 | -1 |
| G: -2104.18652 HOMO: -7.74164 LUMO: 1.37690 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10475.17867 HOMO: -6.98244 LUMO: 1.72520 factor:1 | 1 (-2.43994) | -1 | -1 |
| G: -2104.18652 HOMO: -7.74164 LUMO: 1.37690 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10475.15440 HOMO: -6.37019 LUMO: 2.35923 factor:1 | 1 (-2.41566) | -1 | -1 |
| G: -2104.18652 HOMO: -7.74164 LUMO: 1.37690 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10475.37911 HOMO: -6.55794 LUMO: 2.12521 factor:1 | 1 (-2.64038) | -1 | -1 |
| G: -2104.18652 HOMO: -7.74164 LUMO: 1.37690 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10475.02185 HOMO: -6.45998 LUMO: 1.93201 factor:1 | 1 (-2.28312) | -1 | -1 |
| G: -2104.18652 HOMO: -7.74164 LUMO: 1.37690 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10474.56217 HOMO: -6.71033 LUMO: 1.58370 factor:1 | 1 (-1.82343) | -1 | -1 |
| G: -2104.18652 HOMO: -7.74164 LUMO: 1.37690 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10474.61423 HOMO: -6.67223 LUMO: 1.52928 factor:1 | 1 (-1.87549) | -1 | -1 |
| G: -2104.18652 HOMO: -7.74164 LUMO: 1.37690 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10474.68334 HOMO: -6.72121 LUMO: 1.33608 factor:1 | 1 (-1.94461) | -1 | -1 |
| G: -2104.18652 HOMO: -7.74164 LUMO: 1.37690 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10475.91713 HOMO: -6.89264 LUMO: 2.08983 factor:1 | 1 (-3.17840) | -1 | -1 |
| G: -2104.18652 HOMO: -7.74164 LUMO: 1.37690 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10475.90486 HOMO: -6.31032 LUMO: 2.24766 factor:1 | 1 (-3.16613) | -1 | -1 |
| G: -2104.18652 HOMO: -7.74164 LUMO: 1.37690 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10476.12000 HOMO: -6.79740 LUMO: 2.09528 factor:1 | 1 (-3.38126) | -1 | -1 |
| G: -2104.18652 HOMO: -7.74164 LUMO: 1.37690 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10476.06220 HOMO: -6.78108 LUMO: 2.15786 factor:1 | 1 (-3.32346) | -1 | -1 |
| G: -2104.18652 HOMO: -7.74164 LUMO: 1.37690 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10475.77319 HOMO: -6.50896 LUMO: 2.15786 factor:1 | 1 (-3.03445) | -1 | -1 |
| G: -2104.18652 HOMO: -7.74164 LUMO: 1.37690 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10475.83520 HOMO: -6.56067 LUMO: 2.24494 factor:1 | 1 (-3.09647) | -1 | -1 |
| G: -2104.18652 HOMO: -7.74164 LUMO: 1.37690 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10476.17031 HOMO: -6.72938 LUMO: 2.24494 factor:1 | 1 (-3.43157) | -1 | -1 |
| G: -2104.18652 HOMO: -7.74164 LUMO: 1.37690 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10474.65001 HOMO: -6.40556 LUMO: 1.58642 factor:1 | 1 (-1.91127) | -1 | -1 |
| G: -2104.18652 HOMO: -7.74164 LUMO: 1.37690 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10474.58636 HOMO: -6.63141 LUMO: 1.66262 factor:1 | 1 (-1.84763) | -1 | -1 |
| G: -2104.18652 HOMO: -7.74164 LUMO: 1.37690 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10475.58186 HOMO: -6.97156 LUMO: 2.23678 factor:1 | 1 (-2.84313) | -1 | -1 |
| G: -2104.18652 HOMO: -7.74164 LUMO: 1.37690 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10475.41092 HOMO: -6.86271 LUMO: 1.91296 factor:1 | 1 (-2.67219) | -1 | -1 |
| G: -2104.18652 HOMO: -7.74164 LUMO: 1.37690 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10475.21965 HOMO: -6.50624 LUMO: 1.89119 factor:1 | 1 (-2.48092) | -1 | -1 |
| G: -2104.18652 HOMO: -7.74164 LUMO: 1.37690 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10475.45046 HOMO: -6.70761 LUMO: 1.56193 factor:1 | 1 (-2.71172) | -1 | -1 |
| G: -2104.18652 HOMO: -7.74164 LUMO: 1.37690 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10474.91771 HOMO: -6.60420 LUMO: 1.79595 factor:1 | 1 (-2.17898) | -1 | -1 |
| G: -2104.18652 HOMO: -7.74164 LUMO: 1.37690 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10474.96580 HOMO: -6.85727 LUMO: 2.26943 factor:1 | 1 (-2.22706) | -1 | -1 |
| G: -2104.18652 HOMO: -7.74164 LUMO: 1.37690 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10474.87233 HOMO: -6.23413 LUMO: 1.91024 factor:1 | 1 (-2.13359) | -1 | -1 |
| G: -2104.18652 HOMO: -7.74164 LUMO: 1.37690 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10475.02789 HOMO: -6.84366 LUMO: 2.01364 factor:1 | 1 (-2.28916) | -1 | -1 |
| G: -2104.18652 HOMO: -7.74164 LUMO: 1.37690 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10475.18901 HOMO: -6.63414 LUMO: 2.54971 factor:1 | 1 (-2.45028) | -1 | -1 |
| G: -2104.18652 HOMO: -7.74164 LUMO: 1.37690 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10475.23696 HOMO: -6.52257 LUMO: 2.42998 factor:1 | 1 (-2.49822) | -1 | -1 |
| G: -2104.18652 HOMO: -7.74164 LUMO: 1.37690 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10475.11864 HOMO: -6.61509 LUMO: 2.31297 factor:1 | 1 (-2.37991) | -1 | -1 |
| G: -2104.18652 HOMO: -7.74164 LUMO: 1.37690 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10475.15669 HOMO: -6.45998 LUMO: 2.23405 factor:1 | 1 (-2.41795) | -1 | -1 |
| G: -2104.18652 HOMO: -7.74164 LUMO: 1.37690 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10475.35389 HOMO: -6.86271 LUMO: 2.22317 factor:1 | 1 (-2.61515) | -1 | -1 |
| G: -2104.18652 HOMO: -7.74164 LUMO: 1.37690 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10475.49718 HOMO: -6.84366 LUMO: 2.11432 factor:1 | 1 (-2.75845) | -1 | -1 |
| G: -2104.18652 HOMO: -7.74164 LUMO: 1.37690 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10475.48442 HOMO: -6.85999 LUMO: 2.44902 factor:1 | 1 (-2.74568) | -1 | -1 |
| G: -2104.18652 HOMO: -7.74164 LUMO: 1.37690 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10475.34142 HOMO: -6.73482 LUMO: 1.93745 factor:1 | 1 (-2.60269) | -1 | -1 |
| G: -2104.18652 HOMO: -7.74164 LUMO: 1.37690 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10475.37234 HOMO: -6.91441 LUMO: 2.32385 factor:1 | 1 (-2.63360) | -1 | -1 |
| G: -2104.18652 HOMO: -7.74164 LUMO: 1.37690 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10474.94787 HOMO: -6.16066 LUMO: 2.26399 factor:1 | 1 (-2.20913) | -1 | -1 |
| G: -2104.18652 HOMO: -7.74164 LUMO: 1.37690 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10475.37408 HOMO: -6.71305 LUMO: 2.38644 factor:1 | 1 (-2.63534) | -1 | -1 |
| G: -2104.18652 HOMO: -7.74164 LUMO: 1.37690 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10475.54360 HOMO: -7.08312 LUMO: 2.01636 factor:1 | 1 (-2.80487) | 1 | 1 |
| G: -2104.18652 HOMO: -7.74164 LUMO: 1.37690 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10475.05595 HOMO: -6.15249 LUMO: 1.90752 factor:1 | 1 (-2.31721) | -1 | -1 |
| G: -2104.18652 HOMO: -7.74164 LUMO: 1.37690 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10475.95727 HOMO: -6.83006 LUMO: 2.25855 factor:1 | 1 (-3.21854) | -1 | -1 |
| G: -2104.18652 HOMO: -7.74164 LUMO: 1.37690 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10475.90538 HOMO: -6.77836 LUMO: 2.24766 factor:1 | 1 (-3.16664) | -1 | -1 |
| G: -2104.18652 HOMO: -7.74164 LUMO: 1.37690 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10475.93384 HOMO: -6.66951 LUMO: 2.35923 factor:1 | 1 (-3.19511) | -1 | -1 |
| G: -2104.18652 HOMO: -7.74164 LUMO: 1.37690 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10476.03602 HOMO: -6.68312 LUMO: 2.30208 factor:1 | 1 (-3.29729) | -1 | -1 |
| G: -2104.18652 HOMO: -7.74164 LUMO: 1.37690 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10475.76067 HOMO: -6.49808 LUMO: 2.49801 factor:1 | 1 (-3.02193) | -1 | -1 |
| G: -2104.18652 HOMO: -7.74164 LUMO: 1.37690 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10475.78921 HOMO: -6.62325 LUMO: 1.89935 factor:1 | 1 (-3.05048) | -1 | -1 |
| G: -2104.18652 HOMO: -7.74164 LUMO: 1.37690 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10475.92181 HOMO: -6.80829 LUMO: 1.91296 factor:1 | 1 (-3.18308) | -1 | -1 |
| G: -2104.18652 HOMO: -7.74164 LUMO: 1.37690 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10475.88832 HOMO: -6.64230 LUMO: 2.13065 factor:1 | 1 (-3.14958) | -1 | -1 |
| G: -2104.18652 HOMO: -7.74164 LUMO: 1.37690 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10473.41377 HOMO: -6.40556 LUMO: 1.83949 factor:1 | 1 (-0.67503) | -1 | -1 |
| G: -2104.18652 HOMO: -7.74164 LUMO: 1.37690 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10473.63715 HOMO: -6.48175 LUMO: 1.72248 factor:1 | 1 (-0.89841) | -1 | -1 |
| G: -2104.18652 HOMO: -7.74164 LUMO: 1.37690 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10473.75519 HOMO: -6.61781 LUMO: 2.11432 factor:1 | 1 (-1.01645) | -1 | -1 |
| G: -2104.18652 HOMO: -7.74164 LUMO: 1.37690 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10473.22174 HOMO: -6.34570 LUMO: 2.22317 factor:1 | 1 (-0.48300) | -1 | -1 |
| G: -2104.18652 HOMO: -7.74164 LUMO: 1.37690 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10473.76681 HOMO: -7.00149 LUMO: 1.80139 factor:1 | 1 (-1.02807) | -1 | -1 |
| G: -2104.18652 HOMO: -7.74164 LUMO: 1.37690 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10474.45428 HOMO: -6.66951 LUMO: 2.13065 factor:1 | 1 (-1.71554) | -1 | -1 |
| G: -2104.18652 HOMO: -7.74164 LUMO: 1.37690 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10474.30587 HOMO: -6.54434 LUMO: 2.20140 factor:1 | 1 (-1.56713) | -1 | -1 |
| G: -2104.18652 HOMO: -7.74164 LUMO: 1.37690 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10474.16690 HOMO: -6.67767 LUMO: 2.02997 factor:1 | 1 (-1.42816) | -1 | -1 |
| G: -2104.18652 HOMO: -7.74164 LUMO: 1.37690 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10474.60919 HOMO: -6.49536 LUMO: 2.42998 factor:1 | 1 (-1.87046) | -1 | -1 |
| G: -2104.18652 HOMO: -7.74164 LUMO: 1.37690 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10474.88661 HOMO: -6.70761 LUMO: 2.71025 factor:1 | 1 (-2.14788) | -1 | -1 |
| G: -2104.18652 HOMO: -7.74164 LUMO: 1.37690 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10474.82296 HOMO: -6.62869 LUMO: 2.11160 factor:1 | 1 (-2.08423) | -1 | -1 |
| G: -2104.18652 HOMO: -7.74164 LUMO: 1.37690 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10474.83347 HOMO: -6.61781 LUMO: 2.24494 factor:1 | 1 (-2.09473) | -1 | -1 |
| G: -2104.18652 HOMO: -7.74164 LUMO: 1.37690 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10474.65417 HOMO: -6.66135 LUMO: 2.20956 factor:1 | 1 (-1.91544) | -1 | -1 |
| G: -2104.18652 HOMO: -7.74164 LUMO: 1.37690 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10474.53382 HOMO: -6.95523 LUMO: 2.03813 factor:1 | 1 (-1.79508) | -1 | -1 |
| G: -2104.18652 HOMO: -7.74164 LUMO: 1.37690 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10474.53572 HOMO: -7.11578 LUMO: 2.41365 factor:1 | 1 (-1.79699) | 1 | 1 |
| G: -2104.18652 HOMO: -7.74164 LUMO: 1.37690 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10474.40037 HOMO: -6.99061 LUMO: 2.13881 factor:1 | 1 (-1.66164) | -1 | -1 |
| G: -2104.18652 HOMO: -7.74164 LUMO: 1.37690 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10474.20091 HOMO: -6.43277 LUMO: 2.01364 factor:1 | 1 (-1.46218) | -1 | -1 |
| G: -2104.18652 HOMO: -7.74164 LUMO: 1.37690 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10474.55765 HOMO: -6.79196 LUMO: 2.04358 factor:1 | 1 (-1.81892) | -1 | -1 |
| G: -2104.18652 HOMO: -7.74164 LUMO: 1.37690 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10474.66345 HOMO: -7.08584 LUMO: 1.99732 factor:1 | 1 (-1.92472) | 1 | 1 |
| G: -2104.18652 HOMO: -7.74164 LUMO: 1.37690 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10474.40606 HOMO: -6.46815 LUMO: 2.29936 factor:1 | 1 (-1.66732) | -1 | -1 |
| G: -2104.18652 HOMO: -7.74164 LUMO: 1.37690 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10474.47678 HOMO: -6.78108 LUMO: 1.93745 factor:1 | 1 (-1.73805) | -1 | -1 |
| G: -2104.18652 HOMO: -7.74164 LUMO: 1.37690 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10474.31248 HOMO: -6.43277 LUMO: 1.80956 factor:1 | 1 (-1.57374) | -1 | -1 |
| G: -2104.18652 HOMO: -7.74164 LUMO: 1.37690 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10475.58167 HOMO: -6.71577 LUMO: -0.81090 factor:1 | 1 (-2.84294) | -1 | -1 |
| G: -2104.18652 HOMO: -7.74164 LUMO: 1.37690 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10476.01191 HOMO: -7.14027 LUMO: -0.68028 factor:1 | 1 (-3.27318) | -1 | -1 |
| G: -2104.18652 HOMO: -7.74164 LUMO: 1.37690 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10475.86731 HOMO: -7.03414 LUMO: -0.69661 factor:1 | 1 (-3.12857) | -1 | -1 |
| G: -2104.18652 HOMO: -7.74164 LUMO: 1.37690 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10475.71487 HOMO: -6.64502 LUMO: -0.47348 factor:1 | 1 (-2.97614) | -1 | -1 |
| G: -2104.18652 HOMO: -7.74164 LUMO: 1.37690 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10474.58506 HOMO: -6.60692 LUMO: 2.12793 factor:1 | 1 (-1.84632) | -1 | -1 |
| G: -2104.18652 HOMO: -7.74164 LUMO: 1.37690 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10474.35389 HOMO: -6.66407 LUMO: 1.94561 factor:1 | 1 (-1.61516) | -1 | -1 |
| G: -2104.18652 HOMO: -7.74164 LUMO: 1.37690 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10474.57931 HOMO: -7.10217 LUMO: 1.92384 factor:1 | 1 (-1.84058) | 1 | 1 |
| G: -2104.18652 HOMO: -7.74164 LUMO: 1.37690 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10474.50881 HOMO: -6.84094 LUMO: 1.66534 factor:1 | 1 (-1.77007) | -1 | -1 |
| G: -2104.18652 HOMO: -7.74164 LUMO: 1.37690 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10474.52056 HOMO: -6.93618 LUMO: 2.13065 factor:1 | 1 (-1.78183) | -1 | -1 |
| G: -2104.18652 HOMO: -7.74164 LUMO: 1.37690 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10474.65442 HOMO: -6.60692 LUMO: 2.20684 factor:1 | 1 (-1.91568) | -1 | -1 |
| G: -2104.18652 HOMO: -7.74164 LUMO: 1.37690 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10474.66658 HOMO: -6.85727 LUMO: 2.19324 factor:1 | 1 (-1.92785) | -1 | -1 |
| G: -2104.18652 HOMO: -7.74164 LUMO: 1.37690 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10474.53474 HOMO: -6.31032 LUMO: 1.76330 factor:1 | 1 (-1.79601) | -1 | -1 |
| G: -2104.18652 HOMO: -7.74164 LUMO: 1.37690 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10473.45948 HOMO: -6.43821 LUMO: 2.10072 factor:1 | 1 (-0.72075) | -1 | -1 |
| G: -2104.18652 HOMO: -7.74164 LUMO: 1.37690 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10473.12778 HOMO: -6.42189 LUMO: 2.19596 factor:1 | 1 (-0.38904) | -1 | -1 |
| G: -2104.18652 HOMO: -7.74164 LUMO: 1.37690 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10473.35445 HOMO: -6.40556 LUMO: 2.02181 factor:1 | 1 (-0.61571) | -1 | -1 |
| G: -2104.18652 HOMO: -7.74164 LUMO: 1.37690 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10474.54522 HOMO: -6.41372 LUMO: 2.26671 factor:1 | 1 (-1.80648) | -1 | -1 |
| G: -2104.18652 HOMO: -7.74164 LUMO: 1.37690 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10474.36402 HOMO: -6.60692 LUMO: 2.09800 factor:1 | 1 (-1.62528) | -1 | -1 |
| G: -2104.18652 HOMO: -7.74164 LUMO: 1.37690 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10474.24138 HOMO: -6.75931 LUMO: 1.76602 factor:1 | 1 (-1.50264) | -1 | -1 |
| G: -2104.18652 HOMO: -7.74164 LUMO: 1.37690 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10473.48425 HOMO: -6.39195 LUMO: 1.84221 factor:1 | 1 (-0.74551) | -1 | -1 |
| G: -2104.18652 HOMO: -7.74164 LUMO: 1.37690 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10474.56535 HOMO: -6.74570 LUMO: 2.04085 factor:1 | 1 (-1.82662) | -1 | -1 |
| G: -2104.18652 HOMO: -7.74164 LUMO: 1.37690 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10474.47047 HOMO: -6.77019 LUMO: 2.16875 factor:1 | 1 (-1.73173) | -1 | -1 |
| G: -2104.18652 HOMO: -7.74164 LUMO: 1.37690 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10474.52269 HOMO: -6.15522 LUMO: 1.81772 factor:1 | 1 (-1.78395) | -1 | -1 |
| G: -2104.18652 HOMO: -7.74164 LUMO: 1.37690 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10474.34840 HOMO: -6.48175 LUMO: 2.02453 factor:1 | 1 (-1.60966) | -1 | -1 |
| G: -2104.18652 HOMO: -7.74164 LUMO: 1.37690 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10474.21395 HOMO: -6.57427 LUMO: 1.77962 factor:1 | 1 (-1.47521) | -1 | -1 |
| G: -2104.18652 HOMO: -7.74164 LUMO: 1.37690 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10474.92174 HOMO: -6.57699 LUMO: 2.42998 factor:1 | 1 (-2.18301) | -1 | -1 |
| G: -2104.18652 HOMO: -7.74164 LUMO: 1.37690 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10475.03932 HOMO: -6.35386 LUMO: 2.25310 factor:1 | 1 (-2.30059) | -1 | -1 |
| G: -2104.18652 HOMO: -7.74164 LUMO: 1.37690 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10475.05970 HOMO: -6.80013 LUMO: 2.11160 factor:1 | 1 (-2.32097) | -1 | -1 |
| G: -2104.18652 HOMO: -7.74164 LUMO: 1.37690 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10475.01494 HOMO: -6.24229 LUMO: 2.05718 factor:1 | 1 (-2.27621) | -1 | -1 |
| G: -2104.18652 HOMO: -7.74164 LUMO: 1.37690 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10475.31340 HOMO: -6.42733 LUMO: 1.76874 factor:1 | 1 (-2.57466) | -1 | -1 |
| G: -2104.18652 HOMO: -7.74164 LUMO: 1.37690 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10475.62064 HOMO: -6.56883 LUMO: 2.36195 factor:1 | 1 (-2.88190) | -1 | -1 |
| G: -2104.18652 HOMO: -7.74164 LUMO: 1.37690 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10475.83866 HOMO: -6.72665 LUMO: 2.28848 factor:1 | 1 (-3.09992) | -1 | -1 |
| G: -2104.18652 HOMO: -7.74164 LUMO: 1.37690 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10475.76772 HOMO: -6.39195 LUMO: 1.79051 factor:1 | 1 (-3.02898) | -1 | -1 |
| G: -2104.18652 HOMO: -7.74164 LUMO: 1.37690 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10475.20643 HOMO: -6.70761 LUMO: 0.15510 factor:1 | 1 (-2.46769) | -1 | -1 |
| G: -2104.18652 HOMO: -7.74164 LUMO: 1.37690 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10474.87586 HOMO: -6.44366 LUMO: -0.16871 factor:1 | 1 (-2.13713) | -1 | -1 |
| G: -2104.18652 HOMO: -7.74164 LUMO: 1.37690 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10474.51129 HOMO: -6.68584 LUMO: 1.69527 factor:1 | 1 (-1.77255) | -1 | -1 |
| G: -2104.18652 HOMO: -7.74164 LUMO: 1.37690 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10474.20861 HOMO: -6.26950 LUMO: 1.61636 factor:1 | 1 (-1.46988) | -1 | -1 |
| G: -2104.18652 HOMO: -7.74164 LUMO: 1.37690 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10474.24671 HOMO: -6.47631 LUMO: 1.98915 factor:1 | 1 (-1.50797) | -1 | -1 |
| G: -2104.18652 HOMO: -7.74164 LUMO: 1.37690 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10474.38538 HOMO: -6.58243 LUMO: 1.97283 factor:1 | 1 (-1.64664) | -1 | -1 |
| G: -2104.18652 HOMO: -7.74164 LUMO: 1.37690 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10474.33294 HOMO: -6.51713 LUMO: 1.97283 factor:1 | 1 (-1.59421) | -1 | -1 |
| G: -2104.18652 HOMO: -7.74164 LUMO: 1.37690 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10474.50217 HOMO: -6.65046 LUMO: 1.69255 factor:1 | 1 (-1.76343) | -1 | -1 |
| G: -2104.18652 HOMO: -7.74164 LUMO: 1.37690 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10475.13190 HOMO: -6.26406 LUMO: 2.21773 factor:1 | 1 (-2.39316) | -1 | -1 |
| G: -2104.18652 HOMO: -7.74164 LUMO: 1.37690 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10475.29070 HOMO: -6.88992 LUMO: 2.28304 factor:1 | 1 (-2.55197) | -1 | -1 |
| G: -2104.18652 HOMO: -7.74164 LUMO: 1.37690 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10475.21908 HOMO: -6.67767 LUMO: 2.34834 factor:1 | 1 (-2.48035) | -1 | -1 |
| G: -2104.18652 HOMO: -7.74164 LUMO: 1.37690 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10475.12841 HOMO: -6.52801 LUMO: 2.10344 factor:1 | 1 (-2.38968) | -1 | -1 |
| G: -2104.18652 HOMO: -7.74164 LUMO: 1.37690 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10475.10526 HOMO: -6.52801 LUMO: 2.24222 factor:1 | 1 (-2.36652) | -1 | -1 |
| G: -2104.18652 HOMO: -7.74164 LUMO: 1.37690 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10473.98072 HOMO: -6.17154 LUMO: 1.89663 factor:1 | 1 (-1.24198) | -1 | -1 |
| G: -2104.18652 HOMO: -7.74164 LUMO: 1.37690 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10473.83892 HOMO: -6.42733 LUMO: 2.15514 factor:1 | 1 (-1.10018) | -1 | -1 |
| G: -2104.18652 HOMO: -7.74164 LUMO: 1.37690 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10474.06837 HOMO: -6.36474 LUMO: 2.01364 factor:1 | 1 (-1.32963) | -1 | -1 |
| G: -2104.18652 HOMO: -7.74164 LUMO: 1.37690 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10476.19700 HOMO: -6.82189 LUMO: 1.86942 factor:1 | 1 (-3.45827) | -1 | -1 |
| G: -2104.18652 HOMO: -7.74164 LUMO: 1.37690 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10475.86037 HOMO: -6.60148 LUMO: 2.00548 factor:1 | 1 (-3.12164) | -1 | -1 |
| G: -2104.18652 HOMO: -7.74164 LUMO: 1.37690 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10476.02203 HOMO: -6.67767 LUMO: 2.15786 factor:1 | 1 (-3.28330) | -1 | -1 |
| G: -2104.18652 HOMO: -7.74164 LUMO: 1.37690 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10476.08021 HOMO: -6.79196 LUMO: 2.06534 factor:1 | 1 (-3.34148) | -1 | -1 |
| G: -2104.18652 HOMO: -7.74164 LUMO: 1.37690 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10475.71982 HOMO: -6.70216 LUMO: 1.83405 factor:1 | 1 (-2.98109) | -1 | -1 |
| G: -2104.18652 HOMO: -7.74164 LUMO: 1.37690 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10474.21484 HOMO: -6.58788 LUMO: 1.79051 factor:1 | 1 (-1.47611) | -1 | -1 |
| G: -2104.18652 HOMO: -7.74164 LUMO: 1.37690 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10474.34181 HOMO: -6.34842 LUMO: 1.80139 factor:1 | 1 (-1.60308) | -1 | -1 |
| G: -2104.18652 HOMO: -7.74164 LUMO: 1.37690 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10474.38434 HOMO: -6.48175 LUMO: 1.95922 factor:1 | 1 (-1.64561) | -1 | -1 |
| G: -2104.18652 HOMO: -7.74164 LUMO: 1.37690 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10474.39147 HOMO: -6.71033 LUMO: 2.02997 factor:1 | 1 (-1.65274) | -1 | -1 |
| G: -2104.18652 HOMO: -7.74164 LUMO: 1.37690 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10475.29756 HOMO: -6.89264 LUMO: 2.42726 factor:1 | 1 (-2.55882) | -1 | -1 |
| G: -2104.18652 HOMO: -7.74164 LUMO: 1.37690 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10475.11200 HOMO: -6.74570 LUMO: 2.20684 factor:1 | 1 (-2.37327) | -1 | -1 |
| G: -2104.18652 HOMO: -7.74164 LUMO: 1.37690 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10474.79358 HOMO: -6.30216 LUMO: 2.15242 factor:1 | 1 (-2.05484) | -1 | -1 |
| G: -2104.18652 HOMO: -7.74164 LUMO: 1.37690 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10475.23364 HOMO: -6.94979 LUMO: 2.43814 factor:1 | 1 (-2.49490) | -1 | -1 |
| G: -2104.18652 HOMO: -7.74164 LUMO: 1.37690 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10475.35029 HOMO: -6.97972 LUMO: 2.11432 factor:1 | 1 (-2.61156) | -1 | -1 |
| G: -2104.18652 HOMO: -7.74164 LUMO: 1.37690 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10474.99608 HOMO: -6.17154 LUMO: 1.98099 factor:1 | 1 (-2.25735) | -1 | -1 |
| G: -2104.18652 HOMO: -7.74164 LUMO: 1.37690 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10475.28439 HOMO: -6.74026 LUMO: 2.21501 factor:1 | 1 (-2.54565) | -1 | -1 |
| G: -2104.18652 HOMO: -7.74164 LUMO: 1.37690 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10475.15334 HOMO: -6.72393 LUMO: 2.19596 factor:1 | 1 (-2.41460) | -1 | -1 |
| G: -2104.18652 HOMO: -7.74164 LUMO: 1.37690 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10474.81102 HOMO: -6.11440 LUMO: 2.10072 factor:1 | 1 (-2.07228) | -1 | -1 |
| G: -2104.18652 HOMO: -7.74164 LUMO: 1.37690 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10475.06711 HOMO: -6.34297 LUMO: 1.92657 factor:1 | 1 (-2.32837) | -1 | -1 |
| G: -2104.18652 HOMO: -7.74164 LUMO: 1.37690 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10475.18477 HOMO: -6.24773 LUMO: 2.00276 factor:1 | 1 (-2.44603) | -1 | -1 |
| G: -2104.18652 HOMO: -7.74164 LUMO: 1.37690 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10475.33155 HOMO: -6.75114 LUMO: 1.98643 factor:1 | 1 (-2.59281) | -1 | -1 |
| G: -2104.18652 HOMO: -7.74164 LUMO: 1.37690 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10475.37040 HOMO: -6.69128 LUMO: 2.08711 factor:1 | 1 (-2.63167) | -1 | -1 |
| G: -2104.18652 HOMO: -7.74164 LUMO: 1.37690 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10475.32891 HOMO: -6.65318 LUMO: 2.15514 factor:1 | 1 (-2.59017) | -1 | -1 |
| G: -2104.18652 HOMO: -7.74164 LUMO: 1.37690 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10475.46069 HOMO: -6.67495 LUMO: 1.72248 factor:1 | 1 (-2.72195) | -1 | -1 |
| G: -2104.18652 HOMO: -7.74164 LUMO: 1.37690 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10475.39478 HOMO: -6.58243 LUMO: 1.83405 factor:1 | 1 (-2.65605) | -1 | -1 |
| G: -2104.18652 HOMO: -7.74164 LUMO: 1.37690 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10475.27574 HOMO: -6.61237 LUMO: 1.69799 factor:1 | 1 (-2.53700) | -1 | -1 |
| G: -2104.18652 HOMO: -7.74164 LUMO: 1.37690 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10475.11970 HOMO: -6.57427 LUMO: 2.29936 factor:1 | 1 (-2.38097) | -1 | -1 |
| G: -2104.18652 HOMO: -7.74164 LUMO: 1.37690 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10474.90903 HOMO: -6.40012 LUMO: 2.35378 factor:1 | 1 (-2.17030) | -1 | -1 |
| G: -2104.18652 HOMO: -7.74164 LUMO: 1.37690 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10475.07530 HOMO: -6.90081 LUMO: 2.26671 factor:1 | 1 (-2.33656) | -1 | -1 |
| G: -2104.18652 HOMO: -7.74164 LUMO: 1.37690 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10474.88618 HOMO: -6.44910 LUMO: 2.25855 factor:1 | 1 (-2.14744) | -1 | -1 |
| G: -2104.18652 HOMO: -7.74164 LUMO: 1.37690 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10475.10319 HOMO: -6.61509 LUMO: 2.26943 factor:1 | 1 (-2.36445) | -1 | -1 |
| G: -2104.18652 HOMO: -7.74164 LUMO: 1.37690 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10475.06719 HOMO: -6.78924 LUMO: 2.09256 factor:1 | 1 (-2.32845) | -1 | -1 |
| G: -2104.18652 HOMO: -7.74164 LUMO: 1.37690 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10474.21724 HOMO: -6.47087 LUMO: 1.97555 factor:1 | 1 (-1.47850) | -1 | -1 |
| G: -2104.18652 HOMO: -7.74164 LUMO: 1.37690 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10474.36736 HOMO: -6.75931 LUMO: 1.98643 factor:1 | 1 (-1.62863) | -1 | -1 |
| G: -2104.18652 HOMO: -7.74164 LUMO: 1.37690 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10474.04973 HOMO: -6.17971 LUMO: 2.09800 factor:1 | 1 (-1.31099) | -1 | -1 |
| G: -2104.18652 HOMO: -7.74164 LUMO: 1.37690 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10474.39474 HOMO: -6.83006 LUMO: 1.91840 factor:1 | 1 (-1.65600) | -1 | -1 |
| G: -2104.18652 HOMO: -7.74164 LUMO: 1.37690 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10474.26217 HOMO: -6.72938 LUMO: 2.17419 factor:1 | 1 (-1.52343) | -1 | -1 |
| G: -2104.18652 HOMO: -7.74164 LUMO: 1.37690 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10474.12159 HOMO: -6.78924 LUMO: 2.42726 factor:1 | 1 (-1.38286) | -1 | -1 |
| G: -2104.18652 HOMO: -7.74164 LUMO: 1.37690 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10473.93876 HOMO: -6.41372 LUMO: 1.93745 factor:1 | 1 (-1.20002) | -1 | -1 |
| G: -2104.18652 HOMO: -7.74164 LUMO: 1.37690 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10474.30187 HOMO: -6.85455 LUMO: 2.14970 factor:1 | 1 (-1.56313) | -1 | -1 |
| G: -2104.18652 HOMO: -7.74164 LUMO: 1.37690 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10474.18336 HOMO: -6.38651 LUMO: 2.18507 factor:1 | 1 (-1.44463) | -1 | -1 |
| G: -2104.18652 HOMO: -7.74164 LUMO: 1.37690 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10475.39430 HOMO: -6.81373 LUMO: 2.00548 factor:1 | 1 (-2.65556) | -1 | -1 |
| G: -2104.18652 HOMO: -7.74164 LUMO: 1.37690 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10475.47604 HOMO: -6.64774 LUMO: 2.41365 factor:1 | 1 (-2.73730) | -1 | -1 |
| G: -2104.18652 HOMO: -7.74164 LUMO: 1.37690 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10475.38063 HOMO: -6.70489 LUMO: 2.31569 factor:1 | 1 (-2.64190) | -1 | -1 |
| G: -2104.18652 HOMO: -7.74164 LUMO: 1.37690 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10475.29032 HOMO: -6.49264 LUMO: 1.78779 factor:1 | 1 (-2.55158) | -1 | -1 |
| G: -2104.18652 HOMO: -7.74164 LUMO: 1.37690 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10475.37002 HOMO: -6.81101 LUMO: 1.86670 factor:1 | 1 (-2.63129) | -1 | -1 |
| G: -2104.18652 HOMO: -7.74164 LUMO: 1.37690 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10475.36303 HOMO: -6.72121 LUMO: 1.48846 factor:1 | 1 (-2.62429) | -1 | -1 |
| G: -2104.18652 HOMO: -7.74164 LUMO: 1.37690 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10475.03048 HOMO: -6.35930 LUMO: 1.78507 factor:1 | 1 (-2.29174) | -1 | -1 |
| G: -2104.18652 HOMO: -7.74164 LUMO: 1.37690 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10475.08651 HOMO: -6.38651 LUMO: 2.04358 factor:1 | 1 (-2.34777) | -1 | -1 |
| G: -2104.18652 HOMO: -7.74164 LUMO: 1.37690 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10475.34496 HOMO: -6.42189 LUMO: 1.99187 factor:1 | 1 (-2.60622) | -1 | -1 |
| G: -2104.18652 HOMO: -7.74164 LUMO: 1.37690 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10475.39013 HOMO: -6.69400 LUMO: 1.61091 factor:1 | 1 (-2.65140) | -1 | -1 |
| G: -2104.18652 HOMO: -7.74164 LUMO: 1.37690 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10475.28425 HOMO: -6.81101 LUMO: 2.17419 factor:1 | 1 (-2.54552) | -1 | -1 |
| G: -2104.18652 HOMO: -7.74164 LUMO: 1.37690 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10475.37307 HOMO: -6.90897 LUMO: 2.28576 factor:1 | 1 (-2.63433) | -1 | -1 |
| G: -2104.18652 HOMO: -7.74164 LUMO: 1.37690 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10475.27505 HOMO: -6.75387 LUMO: 2.31297 factor:1 | 1 (-2.53632) | -1 | -1 |
| G: -2104.18652 HOMO: -7.74164 LUMO: 1.37690 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10475.55691 HOMO: -7.05863 LUMO: 2.18780 factor:1 | 1 (-2.81817) | -1 | -1 |
| G: -2104.18652 HOMO: -7.74164 LUMO: 1.37690 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10475.14221 HOMO: -6.56611 LUMO: 1.99187 factor:1 | 1 (-2.40347) | -1 | -1 |
| G: -2104.18652 HOMO: -7.74164 LUMO: 1.37690 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10475.10754 HOMO: -6.59060 LUMO: 1.86398 factor:1 | 1 (-2.36881) | -1 | -1 |
| G: -2104.18652 HOMO: -7.74164 LUMO: 1.37690 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10474.58187 HOMO: -6.59060 LUMO: 1.59459 factor:1 | 1 (-1.84314) | -1 | -1 |
| G: -2104.18652 HOMO: -7.74164 LUMO: 1.37690 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10474.69347 HOMO: -6.57699 LUMO: 1.48030 factor:1 | 1 (-1.95473) | -1 | -1 |
| G: -2104.18652 HOMO: -7.74164 LUMO: 1.37690 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10474.46426 HOMO: -6.99605 LUMO: 2.30208 factor:1 | 1 (-1.72553) | -1 | -1 |
| G: -2104.18652 HOMO: -7.74164 LUMO: 1.37690 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10474.07743 HOMO: -6.42189 LUMO: 2.20412 factor:1 | 1 (-1.33869) | -1 | -1 |
| G: -2104.18652 HOMO: -7.74164 LUMO: 1.37690 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10474.36287 HOMO: -7.15115 LUMO: 1.83405 factor:1 | 1 (-1.62414) | 1 | 1 |
| G: -2104.18652 HOMO: -7.74164 LUMO: 1.37690 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10474.59042 HOMO: -7.08040 LUMO: 2.21773 factor:1 | 1 (-1.85168) | 1 | 1 |
| G: -2104.18652 HOMO: -7.74164 LUMO: 1.37690 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10473.83661 HOMO: -6.72121 LUMO: 1.89663 factor:1 | 1 (-1.09787) | -1 | -1 |
| G: -2104.18652 HOMO: -7.74164 LUMO: 1.37690 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10474.80696 HOMO: -6.25590 LUMO: 1.85037 factor:1 | 1 (-2.06823) | -1 | -1 |
| G: -2104.18652 HOMO: -7.74164 LUMO: 1.37690 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10475.11652 HOMO: -6.70489 LUMO: 1.98915 factor:1 | 1 (-2.37779) | -1 | -1 |
| G: -2104.18652 HOMO: -7.74164 LUMO: 1.37690 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10475.78391 HOMO: -6.53617 LUMO: 2.08439 factor:1 | 1 (-3.04517) | -1 | -1 |
| G: -2104.18652 HOMO: -7.74164 LUMO: 1.37690 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10475.99510 HOMO: -6.69944 LUMO: 1.98915 factor:1 | 1 (-3.25636) | -1 | -1 |
| G: -2104.18652 HOMO: -7.74164 LUMO: 1.37690 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10474.37302 HOMO: -6.79468 LUMO: 1.96466 factor:1 | 1 (-1.63429) | -1 | -1 |
| G: -2104.18652 HOMO: -7.74164 LUMO: 1.37690 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10474.55980 HOMO: -6.79468 LUMO: 1.99459 factor:1 | 1 (-1.82107) | -1 | -1 |
| G: -2104.18652 HOMO: -7.74164 LUMO: 1.37690 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10474.42149 HOMO: -6.58788 LUMO: 1.98371 factor:1 | 1 (-1.68275) | -1 | -1 |
| G: -2104.18652 HOMO: -7.74164 LUMO: 1.37690 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10474.17969 HOMO: -6.58788 LUMO: 2.16603 factor:1 | 1 (-1.44095) | -1 | -1 |
| G: -2104.18652 HOMO: -7.74164 LUMO: 1.37690 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10474.51436 HOMO: -6.56883 LUMO: 1.64085 factor:1 | 1 (-1.77562) | -1 | -1 |
| G: -2104.18652 HOMO: -7.74164 LUMO: 1.37690 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10474.37395 HOMO: -7.19197 LUMO: 2.66127 factor:1 | 1 (-1.63521) | 1 | 1 |
| G: -2104.18652 HOMO: -7.74164 LUMO: 1.37690 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10474.12611 HOMO: -6.48175 LUMO: 2.40004 factor:1 | 1 (-1.38737) | -1 | -1 |
| G: -2104.18652 HOMO: -7.74164 LUMO: 1.37690 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10474.49039 HOMO: -6.18515 LUMO: 2.27759 factor:1 | 1 (-1.75165) | -1 | -1 |
| G: -2104.18652 HOMO: -7.74164 LUMO: 1.37690 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10474.77709 HOMO: -6.64774 LUMO: 2.13337 factor:1 | 1 (-2.03835) | -1 | -1 |
| G: -2104.18652 HOMO: -7.74164 LUMO: 1.37690 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10474.60538 HOMO: -6.39740 LUMO: 1.95106 factor:1 | 1 (-1.86665) | -1 | -1 |
| G: -2104.18652 HOMO: -7.74164 LUMO: 1.37690 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10474.77001 HOMO: -6.59332 LUMO: 1.81772 factor:1 | 1 (-2.03128) | -1 | -1 |
| G: -2104.18652 HOMO: -7.74164 LUMO: 1.37690 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10474.97529 HOMO: -6.68312 LUMO: 2.41909 factor:1 | 1 (-2.23656) | -1 | -1 |
| G: -2104.18652 HOMO: -7.74164 LUMO: 1.37690 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10474.78726 HOMO: -5.87494 LUMO: 2.18235 factor:1 | 1 (-2.04853) | -1 | -1 |
| G: -2104.18652 HOMO: -7.74164 LUMO: 1.37690 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10474.83935 HOMO: -6.30488 LUMO: 2.04902 factor:1 | 1 (-2.10061) | -1 | -1 |
| G: -2104.18652 HOMO: -7.74164 LUMO: 1.37690 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10475.00422 HOMO: -6.65046 LUMO: 2.05446 factor:1 | 1 (-2.26548) | -1 | -1 |
| G: -2104.18652 HOMO: -7.74164 LUMO: 1.37690 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10475.06090 HOMO: -6.55794 LUMO: 2.06807 factor:1 | 1 (-2.32217) | -1 | -1 |
| G: -2104.18652 HOMO: -7.74164 LUMO: 1.37690 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10474.45735 HOMO: -6.68040 LUMO: 1.99187 factor:1 | 1 (-1.71862) | -1 | -1 |
| G: -2104.18652 HOMO: -7.74164 LUMO: 1.37690 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10474.45961 HOMO: -6.60965 LUMO: 2.18780 factor:1 | 1 (-1.72088) | -1 | -1 |
| G: -2104.18652 HOMO: -7.74164 LUMO: 1.37690 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10474.57569 HOMO: -6.88176 LUMO: 2.10344 factor:1 | 1 (-1.83696) | -1 | -1 |
| G: -2104.18652 HOMO: -7.74164 LUMO: 1.37690 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10474.50884 HOMO: -6.63414 LUMO: 1.70615 factor:1 | 1 (-1.77010) | -1 | -1 |
| G: -2104.18652 HOMO: -7.74164 LUMO: 1.37690 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10474.48280 HOMO: -7.15115 LUMO: 2.07351 factor:1 | 1 (-1.74406) | 1 | 1 |
| G: -2104.18652 HOMO: -7.74164 LUMO: 1.37690 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10474.14709 HOMO: -6.85727 LUMO: 2.27759 factor:1 | 1 (-1.40835) | -1 | -1 |
| G: -2104.18652 HOMO: -7.74164 LUMO: 1.37690 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10474.38307 HOMO: -6.91713 LUMO: 2.28848 factor:1 | 1 (-1.64433) | -1 | -1 |
| G: -2104.18652 HOMO: -7.74164 LUMO: 1.37690 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10474.49123 HOMO: -7.10217 LUMO: 2.14698 factor:1 | 1 (-1.75249) | 1 | 1 |
| G: -2104.18652 HOMO: -7.74164 LUMO: 1.37690 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10475.15524 HOMO: -6.78108 LUMO: 2.45447 factor:1 | 1 (-2.41651) | -1 | -1 |
| G: -2104.18652 HOMO: -7.74164 LUMO: 1.37690 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10475.24695 HOMO: -6.78380 LUMO: 2.43542 factor:1 | 1 (-2.50821) | -1 | -1 |
| G: -2104.18652 HOMO: -7.74164 LUMO: 1.37690 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10475.15641 HOMO: -6.60965 LUMO: 2.33474 factor:1 | 1 (-2.41768) | -1 | -1 |
| G: -2104.18652 HOMO: -7.74164 LUMO: 1.37690 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10475.00811 HOMO: -6.72665 LUMO: 2.25855 factor:1 | 1 (-2.26938) | -1 | -1 |
| G: -2104.18652 HOMO: -7.74164 LUMO: 1.37690 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10474.46971 HOMO: -6.27495 LUMO: 2.04358 factor:1 | 1 (-1.73097) | -1 | -1 |
| G: -2104.18652 HOMO: -7.74164 LUMO: 1.37690 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10474.37204 HOMO: -6.17426 LUMO: 1.45853 factor:1 | 1 (-1.63331) | -1 | -1 |
| G: -2104.18652 HOMO: -7.74164 LUMO: 1.37690 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10474.35433 HOMO: -7.21374 LUMO: 2.33474 factor:1 | 1 (-1.61559) | 1 | 1 |
| G: -2104.18652 HOMO: -7.74164 LUMO: 1.37690 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10474.41058 HOMO: -6.94707 LUMO: 1.81772 factor:1 | 1 (-1.67184) | -1 | -1 |
| G: -2542.39370 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -8806.06779 HOMO: -6.80829 LUMO: 0.17960 factor:1 | -1 (0.69160) | -1 | -1 |
| G: -2542.39370 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -8808.59889 HOMO: -7.19469 LUMO: 1.60819 factor:1 | 1 (-1.83949) | 1 | 1 |
| G: -2542.39370 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -8807.90475 HOMO: -6.78652 LUMO: 0.53334 factor:1 | 1 (-1.14535) | -1 | -1 |
| G: -2542.39370 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -8807.60205 HOMO: -6.70489 LUMO: 0.74559 factor:1 | 1 (-0.84265) | -1 | -1 |
| G: -2542.39370 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -8808.05926 HOMO: -6.72393 LUMO: 0.88981 factor:1 | 1 (-1.29986) | -1 | -1 |
| G: -2542.39370 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -8805.99995 HOMO: -4.54430 LUMO: -0.90614 factor:1 | -1 (0.75944) | -1 | -1 |
| G: -2542.39370 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -8808.20301 HOMO: -6.83006 LUMO: 0.47348 factor:1 | 1 (-1.44362) | -1 | -1 |
| G: -2542.39370 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -8808.23967 HOMO: -7.07496 LUMO: 0.50613 factor:1 | 1 (-1.48027) | -1 | -1 |
| G: -2542.39370 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -8807.70306 HOMO: -6.62053 LUMO: 0.74559 factor:1 | 1 (-0.94366) | -1 | -1 |
| G: -2542.39370 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -8808.35869 HOMO: -6.79196 LUMO: 1.80139 factor:1 | 1 (-1.59929) | -1 | -1 |
| G: -2542.39370 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -8807.89351 HOMO: -6.71033 LUMO: 0.40817 factor:1 | 1 (-1.13412) | -1 | -1 |
| G: -2542.39370 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -8807.73895 HOMO: -6.74026 LUMO: 0.95784 factor:1 | 1 (-0.97956) | -1 | -1 |
| G: -2542.39370 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -8806.87341 HOMO: -7.34707 LUMO: 0.40001 factor:1 | 1 (-0.11402) | -1 | -1 |
| G: -2542.39370 HOMO: -9.80698 LUMO: 0.51974 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11347.77563 HOMO: -6.19875 LUMO: -0.88709 factor:1 | -1 (1.37747) | -1 | -1 |
| G: -2542.39370 HOMO: -9.80698 LUMO: 0.51974 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11349.74130 HOMO: -6.48719 LUMO: -0.14694 factor:1 | 1 (-0.58820) | -1 | -1 |
| G: -2542.39370 HOMO: -9.80698 LUMO: 0.51974 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11349.42031 HOMO: -6.73482 LUMO: -0.01633 factor:1 | 1 (-0.26722) | -1 | -1 |
| G: -2542.39370 HOMO: -9.80698 LUMO: 0.51974 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11348.45668 HOMO: -7.05591 LUMO: -0.20136 factor:1 | -1 (0.69642) | -1 | -1 |
| G: -2542.39370 HOMO: -9.80698 LUMO: 0.51974 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11347.84200 HOMO: -6.38651 LUMO: -2.07895 factor:1 | -1 (1.31110) | -1 | -1 |
| G: -2542.39370 HOMO: -9.80698 LUMO: 0.51974 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11349.74416 HOMO: -6.85455 LUMO: -1.03403 factor:1 | 1 (-0.59106) | -1 | -1 |
| G: -2542.39370 HOMO: -9.80698 LUMO: 0.51974 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11349.66873 HOMO: -6.72121 LUMO: -0.99322 factor:1 | 1 (-0.51563) | -1 | -1 |
| G: -2542.39370 HOMO: -9.80698 LUMO: 0.51974 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11347.46994 HOMO: -6.53890 LUMO: -0.10885 factor:1 | -1 (1.68316) | -1 | -1 |
| G: -2542.39370 HOMO: -9.80698 LUMO: 0.51974 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11351.12111 HOMO: -6.68312 LUMO: 0.21225 factor:1 | 1 (-1.96801) | -1 | -1 |
| G: -2542.39370 HOMO: -9.80698 LUMO: 0.51974 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11351.12130 HOMO: -6.68040 LUMO: 0.21225 factor:1 | 1 (-1.96820) | -1 | -1 |
| G: -2542.39370 HOMO: -9.80698 LUMO: 0.51974 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11351.45845 HOMO: -6.76475 LUMO: -0.64491 factor:1 | 1 (-2.30535) | -1 | -1 |
| G: -2542.39370 HOMO: -9.80698 LUMO: 0.51974 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11351.79143 HOMO: -6.48175 LUMO: 0.41633 factor:1 | 1 (-2.63833) | -1 | -1 |
| G: -2542.39370 HOMO: -9.80698 LUMO: 0.51974 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11351.20919 HOMO: -6.42733 LUMO: 0.16599 factor:1 | 1 (-2.05609) | -1 | -1 |
| G: -2542.39370 HOMO: -9.80698 LUMO: 0.51974 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11351.77184 HOMO: -6.66679 LUMO: 0.77825 factor:1 | 1 (-2.61874) | -1 | -1 |
| G: -2542.39370 HOMO: -9.80698 LUMO: 0.51974 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11351.09931 HOMO: -6.75931 LUMO: -0.73471 factor:1 | 1 (-1.94621) | -1 | -1 |
| G: -2542.39370 HOMO: -9.80698 LUMO: 0.51974 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11351.19069 HOMO: -6.53617 LUMO: 0.38096 factor:1 | 1 (-2.03759) | -1 | -1 |
| G: -2542.39370 HOMO: -9.80698 LUMO: 0.51974 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11350.43579 HOMO: -6.34297 LUMO: 0.35375 factor:1 | 1 (-1.28269) | -1 | -1 |
| G: -2542.39370 HOMO: -9.80698 LUMO: 0.51974 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11351.11436 HOMO: -7.11850 LUMO: -0.03265 factor:1 | 1 (-1.96126) | -1 | -1 |
| G: -2542.39370 HOMO: -9.80698 LUMO: 0.51974 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11351.15371 HOMO: -5.21914 LUMO: 1.29798 factor:1 | 1 (-2.00061) | -1 | -1 |
| G: -2542.39370 HOMO: -9.80698 LUMO: 0.51974 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11350.73283 HOMO: -7.09129 LUMO: -0.66668 factor:1 | 1 (-1.57973) | -1 | -1 |
| G: -2542.39370 HOMO: -9.80698 LUMO: 0.51974 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11350.75949 HOMO: -6.96884 LUMO: -0.31021 factor:1 | 1 (-1.60640) | -1 | -1 |
| G: -2542.39370 HOMO: -9.80698 LUMO: 0.51974 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11351.15395 HOMO: -6.51713 LUMO: -0.59865 factor:1 | 1 (-2.00085) | -1 | -1 |
| G: -2542.39370 HOMO: -9.80698 LUMO: 0.51974 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11351.67407 HOMO: -6.69400 LUMO: -0.07075 factor:1 | 1 (-2.52097) | -1 | -1 |
| G: -2542.39370 HOMO: -9.80698 LUMO: 0.51974 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11351.18908 HOMO: -5.28173 LUMO: 1.17281 factor:1 | 1 (-2.03598) | -1 | -1 |
| G: -2542.39370 HOMO: -9.80698 LUMO: 0.51974 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11351.70683 HOMO: -6.54434 LUMO: 0.32109 factor:1 | 1 (-2.55373) | -1 | -1 |
| G: -2542.39370 HOMO: -9.80698 LUMO: 0.51974 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11352.03957 HOMO: -6.79740 LUMO: -0.24762 factor:1 | 1 (-2.88647) | -1 | -1 |
| G: -2542.39370 HOMO: -9.80698 LUMO: 0.51974 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11351.04108 HOMO: -6.91986 LUMO: -0.14694 factor:1 | 1 (-1.88798) | -1 | -1 |
| G: -2542.39370 HOMO: -9.80698 LUMO: 0.51974 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11350.94284 HOMO: -6.75114 LUMO: 0.18504 factor:1 | 1 (-1.78975) | -1 | -1 |
| G: -2542.39370 HOMO: -9.80698 LUMO: 0.51974 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11351.40538 HOMO: -6.74842 LUMO: 0.69389 factor:1 | 1 (-2.25229) | -1 | -1 |
| G: -2542.39370 HOMO: -9.80698 LUMO: 0.51974 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11350.59653 HOMO: -7.01782 LUMO: 0.56600 factor:1 | 1 (-1.44343) | -1 | -1 |
| G: -2542.39370 HOMO: -9.80698 LUMO: 0.51974 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11350.41976 HOMO: -6.47359 LUMO: -0.56600 factor:1 | 1 (-1.26666) | -1 | -1 |
| G: -2542.39370 HOMO: -9.80698 LUMO: 0.51974 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11350.99177 HOMO: -6.63686 LUMO: -0.55783 factor:1 | 1 (-1.83867) | -1 | -1 |
| G: -2542.39370 HOMO: -9.80698 LUMO: 0.51974 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11349.03633 HOMO: -4.13885 LUMO: -2.05446 factor:1 | -1 (0.11676) | -1 | -1 |
| G: -2542.39370 HOMO: -9.80698 LUMO: 0.51974 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11350.72951 HOMO: -6.34570 LUMO: 0.19864 factor:1 | 1 (-1.57641) | -1 | -1 |
| G: -2542.39370 HOMO: -9.80698 LUMO: 0.51974 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11350.25440 HOMO: -6.47903 LUMO: 0.24762 factor:1 | 1 (-1.10130) | -1 | -1 |
| G: -2542.39370 HOMO: -9.80698 LUMO: 0.51974 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11350.00702 HOMO: -6.15249 LUMO: 0.32109 factor:1 | 1 (-0.85392) | -1 | -1 |
| G: -2542.39370 HOMO: -9.80698 LUMO: 0.51974 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11350.94372 HOMO: -6.84366 LUMO: 0.29116 factor:1 | 1 (-1.79062) | -1 | -1 |
| G: -2542.39370 HOMO: -9.80698 LUMO: 0.51974 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11350.72953 HOMO: -6.34297 LUMO: 0.19864 factor:1 | 1 (-1.57644) | -1 | -1 |
| G: -2542.39370 HOMO: -9.80698 LUMO: 0.51974 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11350.28534 HOMO: -6.51168 LUMO: 0.30749 factor:1 | 1 (-1.13224) | -1 | -1 |
| G: -2542.39370 HOMO: -9.80698 LUMO: 0.51974 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11351.34503 HOMO: -6.79468 LUMO: -0.16599 factor:1 | 1 (-2.19193) | -1 | -1 |
| G: -2542.39370 HOMO: -9.80698 LUMO: 0.51974 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11351.02418 HOMO: -7.24095 LUMO: 0.15238 factor:1 | 1 (-1.87108) | -1 | -1 |
| G: -2542.39370 HOMO: -9.80698 LUMO: 0.51974 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11350.83199 HOMO: -7.06952 LUMO: -0.34558 factor:1 | 1 (-1.67889) | -1 | -1 |
| G: -2542.39370 HOMO: -9.80698 LUMO: 0.51974 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11350.84790 HOMO: -6.88176 LUMO: 0.02177 factor:1 | 1 (-1.69481) | -1 | -1 |
| G: -2542.39370 HOMO: -9.80698 LUMO: 0.51974 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11350.15970 HOMO: -6.37291 LUMO: -0.69117 factor:1 | 1 (-1.00660) | -1 | -1 |
| G: -2542.39370 HOMO: -9.80698 LUMO: 0.51974 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11350.18191 HOMO: -6.83278 LUMO: -0.59049 factor:1 | 1 (-1.02881) | -1 | -1 |
| G: -2542.39370 HOMO: -9.80698 LUMO: 0.51974 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11349.79153 HOMO: -6.57155 LUMO: -0.33470 factor:1 | 1 (-0.63843) | -1 | -1 |
| G: -2542.39370 HOMO: -9.80698 LUMO: 0.51974 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11350.37739 HOMO: -6.89537 LUMO: -0.58504 factor:1 | 1 (-1.22429) | -1 | -1 |
| G: -2542.39370 HOMO: -9.80698 LUMO: 0.51974 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11350.22670 HOMO: -6.57155 LUMO: -0.34831 factor:1 | 1 (-1.07360) | -1 | -1 |
| G: -2542.39370 HOMO: -9.80698 LUMO: 0.51974 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11350.81958 HOMO: -6.64774 LUMO: -0.95784 factor:1 | 1 (-1.66648) | -1 | -1 |
| G: -2542.39370 HOMO: -9.80698 LUMO: 0.51974 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11350.45369 HOMO: -6.91713 LUMO: -0.69933 factor:1 | 1 (-1.30060) | -1 | -1 |
| G: -2542.39370 HOMO: -9.80698 LUMO: 0.51974 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11350.57255 HOMO: -6.80557 LUMO: -0.65035 factor:1 | 1 (-1.41945) | -1 | -1 |
| G: -2542.39370 HOMO: -9.80698 LUMO: 0.51974 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11350.74235 HOMO: -7.26544 LUMO: -0.79729 factor:1 | 1 (-1.58925) | -1 | -1 |
| G: -2542.39370 HOMO: -9.80698 LUMO: 0.51974 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11351.01166 HOMO: -6.69128 LUMO: -0.16871 factor:1 | 1 (-1.85856) | -1 | -1 |
| G: -2542.39370 HOMO: -9.80698 LUMO: 0.51974 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11350.74423 HOMO: -6.88448 LUMO: 0.13061 factor:1 | 1 (-1.59113) | -1 | -1 |
| G: -2542.39370 HOMO: -9.80698 LUMO: 0.51974 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11350.95691 HOMO: -6.50352 LUMO: 0.12245 factor:1 | 1 (-1.80382) | -1 | -1 |
| G: -2542.39370 HOMO: -9.80698 LUMO: 0.51974 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11351.50130 HOMO: -6.56067 LUMO: 0.17687 factor:1 | 1 (-2.34821) | -1 | -1 |
| G: -2542.39370 HOMO: -9.80698 LUMO: 0.51974 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11350.64730 HOMO: -6.70216 LUMO: 0.25034 factor:1 | 1 (-1.49420) | -1 | -1 |
| G: -2542.39370 HOMO: -9.80698 LUMO: 0.51974 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11350.76992 HOMO: -6.51713 LUMO: -0.78369 factor:1 | 1 (-1.61682) | -1 | -1 |
| G: -2542.39370 HOMO: -9.80698 LUMO: 0.51974 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11350.95694 HOMO: -6.50352 LUMO: 0.12245 factor:1 | 1 (-1.80384) | -1 | -1 |
| G: -2542.39370 HOMO: -9.80698 LUMO: 0.51974 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11351.02783 HOMO: -6.22052 LUMO: -0.83811 factor:1 | 1 (-1.87473) | -1 | -1 |
| G: -2542.39370 HOMO: -9.80698 LUMO: 0.51974 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11351.80724 HOMO: -6.51168 LUMO: -0.76464 factor:1 | 1 (-2.65414) | -1 | -1 |
| G: -2542.39370 HOMO: -9.80698 LUMO: 0.51974 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11350.95191 HOMO: -7.14571 LUMO: -0.80274 factor:1 | 1 (-1.79881) | -1 | -1 |
| G: -2542.39370 HOMO: -9.80698 LUMO: 0.51974 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11350.79645 HOMO: -6.66679 LUMO: -0.88709 factor:1 | 1 (-1.64335) | -1 | -1 |
| G: -2542.39370 HOMO: -9.80698 LUMO: 0.51974 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11349.85474 HOMO: -6.76203 LUMO: -1.43948 factor:1 | 1 (-0.70165) | -1 | -1 |
| G: -2542.39370 HOMO: -9.80698 LUMO: 0.51974 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11350.13739 HOMO: -6.57427 LUMO: -1.62996 factor:1 | 1 (-0.98429) | -1 | -1 |
| G: -2542.39370 HOMO: -9.80698 LUMO: 0.51974 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11351.47850 HOMO: -5.05043 LUMO: 1.24900 factor:1 | 1 (-2.32540) | -1 | -1 |
| G: -2542.39370 HOMO: -9.80698 LUMO: 0.51974 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11351.80223 HOMO: -6.53345 LUMO: 0.23130 factor:1 | 1 (-2.64914) | -1 | -1 |
| G: -2542.39370 HOMO: -9.80698 LUMO: 0.51974 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11351.83323 HOMO: -7.18381 LUMO: -0.22585 factor:1 | 1 (-2.68013) | -1 | -1 |
| G: -2542.39370 HOMO: -9.80698 LUMO: 0.51974 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11350.36006 HOMO: -7.00965 LUMO: -1.79595 factor:1 | 1 (-1.20696) | -1 | -1 |
| G: -2542.39370 HOMO: -9.80698 LUMO: 0.51974 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11350.56227 HOMO: -6.08174 LUMO: -0.82995 factor:1 | 1 (-1.40917) | -1 | -1 |
| G: -2542.39370 HOMO: -9.80698 LUMO: 0.51974 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11351.35001 HOMO: -6.42189 LUMO: -0.84355 factor:1 | 1 (-2.19691) | -1 | -1 |
| G: -2542.39370 HOMO: -9.80698 LUMO: 0.51974 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11349.69450 HOMO: -6.53890 LUMO: 0.60409 factor:1 | 1 (-0.54140) | -1 | -1 |
| G: -2542.39370 HOMO: -9.80698 LUMO: 0.51974 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11349.73678 HOMO: -6.62869 LUMO: 0.43810 factor:1 | 1 (-0.58368) | -1 | -1 |
| G: -2542.39370 HOMO: -9.80698 LUMO: 0.51974 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11350.07118 HOMO: -6.68312 LUMO: 0.64491 factor:1 | 1 (-0.91808) | -1 | -1 |
| G: -2542.39370 HOMO: -9.80698 LUMO: 0.51974 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11350.05945 HOMO: -6.42189 LUMO: 1.51295 factor:1 | 1 (-0.90636) | -1 | -1 |
| G: -2542.39370 HOMO: -9.80698 LUMO: 0.51974 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11350.04781 HOMO: -6.17971 LUMO: 1.67622 factor:1 | 1 (-0.89471) | -1 | -1 |
| G: -2542.39370 HOMO: -9.80698 LUMO: 0.51974 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11350.00128 HOMO: -6.79196 LUMO: 1.36873 factor:1 | 1 (-0.84818) | -1 | -1 |
| G: -2542.39370 HOMO: -9.80698 LUMO: 0.51974 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11349.41533 HOMO: -7.38517 LUMO: 0.56328 factor:1 | 1 (-0.26224) | 1 | 1 |
| G: -2542.39370 HOMO: -9.80698 LUMO: 0.51974 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11349.56312 HOMO: -7.56204 LUMO: 0.71566 factor:1 | 1 (-0.41002) | 1 | 1 |
| G: -2542.39370 HOMO: -9.80698 LUMO: 0.51974 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11350.11861 HOMO: -6.45726 LUMO: -1.91840 factor:1 | 1 (-0.96551) | -1 | -1 |
| G: -2542.39370 HOMO: -9.80698 LUMO: 0.51974 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11350.70758 HOMO: -6.13073 LUMO: -0.97417 factor:1 | 1 (-1.55448) | -1 | -1 |
| G: -2542.39370 HOMO: -9.80698 LUMO: 0.51974 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11351.65361 HOMO: -6.50352 LUMO: -0.69661 factor:1 | 1 (-2.50051) | -1 | -1 |
| G: -2542.39370 HOMO: -9.80698 LUMO: 0.51974 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11350.17274 HOMO: -6.76747 LUMO: -1.71976 factor:1 | 1 (-1.01964) | -1 | -1 |
| G: -2542.39370 HOMO: -9.80698 LUMO: 0.51974 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11350.54455 HOMO: -6.48447 LUMO: -0.89525 factor:1 | 1 (-1.39145) | -1 | -1 |
| G: -2542.39370 HOMO: -9.80698 LUMO: 0.51974 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11350.46548 HOMO: -7.11850 LUMO: -0.71566 factor:1 | 1 (-1.31238) | -1 | -1 |
| G: -2542.39370 HOMO: -9.80698 LUMO: 0.51974 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11350.19018 HOMO: -6.80285 LUMO: -0.49253 factor:1 | 1 (-1.03708) | -1 | -1 |
| G: -2542.39370 HOMO: -9.80698 LUMO: 0.51974 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11350.89416 HOMO: -6.80557 LUMO: -0.88165 factor:1 | 1 (-1.74107) | -1 | -1 |
| G: -2542.39370 HOMO: -9.80698 LUMO: 0.51974 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11351.40228 HOMO: -6.94162 LUMO: -0.08980 factor:1 | 1 (-2.24918) | -1 | -1 |
| G: -2542.39370 HOMO: -9.80698 LUMO: 0.51974 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11350.45315 HOMO: -6.97972 LUMO: -0.29388 factor:1 | 1 (-1.30005) | -1 | -1 |
| G: -2542.39370 HOMO: -9.80698 LUMO: 0.51974 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11350.86543 HOMO: -6.75114 LUMO: 0.04626 factor:1 | 1 (-1.71233) | -1 | -1 |
| G: -2542.39370 HOMO: -9.80698 LUMO: 0.51974 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11349.38325 HOMO: -7.15932 LUMO: 0.68845 factor:1 | 1 (-0.23015) | 1 | 1 |
| G: -2542.39370 HOMO: -9.80698 LUMO: 0.51974 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11349.50097 HOMO: -7.36612 LUMO: 0.63675 factor:1 | 1 (-0.34787) | 1 | 1 |
| G: -2542.39370 HOMO: -9.80698 LUMO: 0.51974 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11350.52768 HOMO: -7.02598 LUMO: -0.66124 factor:1 | 1 (-1.37458) | -1 | -1 |
| G: -2542.39370 HOMO: -9.80698 LUMO: 0.51974 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11350.31021 HOMO: -6.89264 LUMO: -0.54967 factor:1 | 1 (-1.15711) | -1 | -1 |
| G: -2542.39370 HOMO: -9.80698 LUMO: 0.51974 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11350.84086 HOMO: -6.97700 LUMO: 0.27756 factor:1 | 1 (-1.68776) | -1 | -1 |
| G: -2542.39370 HOMO: -9.80698 LUMO: 0.51974 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11350.65155 HOMO: -6.60965 LUMO: 0.08163 factor:1 | 1 (-1.49845) | -1 | -1 |
| G: -2542.39370 HOMO: -9.80698 LUMO: 0.51974 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11351.35197 HOMO: -6.70761 LUMO: 0.40001 factor:1 | 1 (-2.19887) | -1 | -1 |
| G: -2542.39370 HOMO: -9.80698 LUMO: 0.51974 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11350.25012 HOMO: -6.69128 LUMO: 0.23674 factor:1 | 1 (-1.09703) | -1 | -1 |
| G: -2542.39370 HOMO: -9.80698 LUMO: 0.51974 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11350.84986 HOMO: -6.69128 LUMO: -0.69933 factor:1 | 1 (-1.69677) | -1 | -1 |
| G: -2542.39370 HOMO: -9.80698 LUMO: 0.51974 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11350.01320 HOMO: -6.18515 LUMO: -0.85988 factor:1 | 1 (-0.86010) | -1 | -1 |
| G: -2542.39370 HOMO: -9.80698 LUMO: 0.51974 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11349.95121 HOMO: -6.86815 LUMO: -1.90208 factor:1 | 1 (-0.79811) | -1 | -1 |
| G: -2542.39370 HOMO: -9.80698 LUMO: 0.51974 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11349.74380 HOMO: -6.37563 LUMO: -1.74697 factor:1 | 1 (-0.59070) | -1 | -1 |
| G: -2542.39370 HOMO: -9.80698 LUMO: 0.51974 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11349.21672 HOMO: -6.75659 LUMO: 0.36463 factor:1 | 1 (-0.06362) | -1 | -1 |
| G: -2542.39370 HOMO: -9.80698 LUMO: 0.51974 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11350.25453 HOMO: -6.91441 LUMO: -0.88981 factor:1 | 1 (-1.10144) | -1 | -1 |
| G: -2542.39370 HOMO: -9.80698 LUMO: 0.51974 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11350.28773 HOMO: -6.71305 LUMO: -0.29933 factor:1 | 1 (-1.13463) | -1 | -1 |
| G: -2542.39370 HOMO: -9.80698 LUMO: 0.51974 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11350.28808 HOMO: -6.91441 LUMO: -1.04492 factor:1 | 1 (-1.13499) | -1 | -1 |
| G: -2542.39370 HOMO: -9.80698 LUMO: 0.51974 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11350.62006 HOMO: -6.05453 LUMO: -0.83539 factor:1 | 1 (-1.46697) | -1 | -1 |
| G: -2542.39370 HOMO: -9.80698 LUMO: 0.51974 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11351.73298 HOMO: -7.35252 LUMO: -0.45715 factor:1 | 1 (-2.57988) | -1 | -1 |
| G: -2542.39370 HOMO: -9.80698 LUMO: 0.51974 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11350.57459 HOMO: -6.41644 LUMO: -0.97417 factor:1 | 1 (-1.42150) | -1 | -1 |
| G: -2542.39370 HOMO: -9.80698 LUMO: 0.51974 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11349.80729 HOMO: -6.78924 LUMO: 0.36735 factor:1 | 1 (-0.65419) | -1 | -1 |
| G: -2542.39370 HOMO: -9.80698 LUMO: 0.51974 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11349.63428 HOMO: -6.74298 LUMO: 0.51974 factor:1 | 1 (-0.48118) | -1 | -1 |
| G: -2542.39370 HOMO: -9.80698 LUMO: 0.51974 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11350.84709 HOMO: -6.48992 LUMO: 1.44765 factor:1 | 1 (-1.69399) | -1 | -1 |
| G: -2542.39370 HOMO: -9.80698 LUMO: 0.51974 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11350.16928 HOMO: -6.12528 LUMO: 1.57826 factor:1 | 1 (-1.01618) | -1 | -1 |
| G: -2542.39370 HOMO: -9.80698 LUMO: 0.51974 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11350.81090 HOMO: -6.62325 LUMO: 1.57826 factor:1 | 1 (-1.65780) | -1 | -1 |
| G: -2542.39370 HOMO: -9.80698 LUMO: 0.51974 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11350.17393 HOMO: -6.19875 LUMO: 1.29798 factor:1 | 1 (-1.02084) | -1 | -1 |
| G: -2542.39370 HOMO: -9.80698 LUMO: 0.51974 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11350.04473 HOMO: -6.74570 LUMO: 1.52112 factor:1 | 1 (-0.89164) | -1 | -1 |
| G: -2542.39370 HOMO: -9.80698 LUMO: 0.51974 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11350.00217 HOMO: -6.84094 LUMO: 1.48574 factor:1 | 1 (-0.84908) | -1 | -1 |
| G: -2542.39370 HOMO: -9.80698 LUMO: 0.51974 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11349.15693 HOMO: -6.85183 LUMO: 0.33470 factor:1 | 1 (-0.00384) | -1 | -1 |
| G: -2542.39370 HOMO: -9.80698 LUMO: 0.51974 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11348.98384 HOMO: -6.51168 LUMO: 0.48164 factor:1 | -1 (0.16925) | -1 | -1 |
| G: -2542.39370 HOMO: -9.80698 LUMO: 0.51974 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11349.59926 HOMO: -6.25046 LUMO: 0.75648 factor:1 | 1 (-0.44616) | -1 | -1 |
| G: -2542.39370 HOMO: -9.80698 LUMO: 0.51974 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11349.80029 HOMO: -6.65591 LUMO: 0.32109 factor:1 | 1 (-0.64720) | -1 | -1 |
| G: -2542.39370 HOMO: -9.80698 LUMO: 0.51974 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11349.54260 HOMO: -6.71033 LUMO: 0.40817 factor:1 | 1 (-0.38950) | -1 | -1 |
| G: -2542.39370 HOMO: -9.80698 LUMO: 0.51974 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11349.88854 HOMO: -6.75114 LUMO: 0.73471 factor:1 | 1 (-0.73544) | -1 | -1 |
| G: -2542.39370 HOMO: -9.80698 LUMO: 0.51974 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11349.73746 HOMO: -6.50624 LUMO: 0.59321 factor:1 | 1 (-0.58436) | -1 | -1 |
| G: -2542.39370 HOMO: -9.80698 LUMO: 0.51974 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11349.71226 HOMO: -6.39740 LUMO: 0.83267 factor:1 | 1 (-0.55917) | -1 | -1 |
| G: -2542.39370 HOMO: -9.80698 LUMO: 0.51974 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11349.86672 HOMO: -6.44094 LUMO: 0.65579 factor:1 | 1 (-0.71362) | -1 | -1 |
| G: -2542.39370 HOMO: -9.80698 LUMO: 0.51974 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11350.38923 HOMO: -6.52257 LUMO: 0.05714 factor:1 | 1 (-1.23613) | -1 | -1 |
| G: -2542.39370 HOMO: -9.80698 LUMO: 0.51974 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11349.30238 HOMO: -7.10217 LUMO: 0.49797 factor:1 | 1 (-0.14928) | -1 | -1 |
| G: -2542.39370 HOMO: -9.80698 LUMO: 0.51974 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11351.06728 HOMO: -6.83006 LUMO: 0.55783 factor:1 | 1 (-1.91418) | -1 | -1 |
| G: -2542.39370 HOMO: -9.80698 LUMO: 0.51974 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11350.28308 HOMO: -6.99333 LUMO: -0.79457 factor:1 | 1 (-1.12998) | -1 | -1 |
| G: -2542.39370 HOMO: -9.80698 LUMO: 0.51974 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11349.71414 HOMO: -6.64230 LUMO: 0.32382 factor:1 | 1 (-0.56104) | -1 | -1 |
| G: -2542.39370 HOMO: -9.80698 LUMO: 0.51974 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11349.57991 HOMO: -6.90897 LUMO: 0.30749 factor:1 | 1 (-0.42681) | -1 | -1 |
| G: -3115.84705 HOMO: -7.26544 LUMO: -1.10478 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -9380.30507 HOMO: -7.09129 LUMO: 1.33336 factor:1 | 1 (-0.09233) | 1 | 1 |
| G: -3115.84705 HOMO: -7.26544 LUMO: -1.10478 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12496.28083 HOMO: -6.66951 LUMO: 1.34424 factor:1 | 1 (-0.22104) | -1 | -1 |
| G: -3115.84705 HOMO: -7.26544 LUMO: -1.10478 factor:2 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12496.27218 HOMO: -7.02870 LUMO: 1.48574 factor:1 | 1 (-0.21238) | -1 | -1 |
| G: -3173.76668 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -9440.25605 HOMO: -7.26544 LUMO: 0.32926 factor:1 | 1 (-2.12369) | -1 | -1 |
| G: -3173.76668 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -9439.74396 HOMO: -6.56067 LUMO: -0.45987 factor:1 | 1 (-1.61159) | -1 | -1 |
| G: -3173.76668 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -9440.07989 HOMO: -6.54434 LUMO: -0.28300 factor:1 | 1 (-1.94752) | -1 | -1 |
| G: -3173.76668 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -9440.77998 HOMO: -7.19469 LUMO: 0.54695 factor:1 | 1 (-2.64761) | -1 | -1 |
| G: -3173.76668 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -9439.97836 HOMO: -6.47359 LUMO: -0.22041 factor:1 | 1 (-1.84599) | -1 | -1 |
| G: -3173.76668 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -9438.92939 HOMO: -6.80013 LUMO: 2.08167 factor:1 | 1 (-0.79702) | -1 | -1 |
| G: -3173.76668 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -9438.91840 HOMO: -6.23957 LUMO: 1.67894 factor:1 | 1 (-0.78603) | -1 | -1 |
| G: -3173.76668 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -9439.55718 HOMO: -6.75114 LUMO: -0.62858 factor:1 | 1 (-1.42482) | -1 | -1 |
| G: -3173.76668 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -9439.69207 HOMO: -6.79468 LUMO: -0.64491 factor:1 | 1 (-1.55970) | -1 | -1 |
| G: -3173.76668 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -9439.41781 HOMO: -6.84911 LUMO: -0.69661 factor:1 | 1 (-1.28544) | -1 | -1 |
| G: -3173.76668 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -9440.17540 HOMO: -7.54028 LUMO: 0.25851 factor:1 | 1 (-2.04303) | -1 | -1 |
| G: -3173.76668 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -9439.45384 HOMO: -6.92802 LUMO: -0.71022 factor:1 | 1 (-1.32147) | -1 | -1 |
| G: -3173.76668 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -9439.66900 HOMO: -6.72665 LUMO: -0.46804 factor:1 | 1 (-1.53663) | -1 | -1 |
| G: -3173.76668 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -9439.87202 HOMO: -6.63686 LUMO: -0.23674 factor:1 | 1 (-1.73965) | -1 | -1 |
| G: -3173.76668 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -9440.66017 HOMO: -7.21102 LUMO: 0.54423 factor:1 | 1 (-2.52780) | -1 | -1 |
| G: -3173.76668 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -9439.64603 HOMO: -6.63414 LUMO: -0.25034 factor:1 | 1 (-1.51366) | -1 | -1 |
| G: -3173.76668 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -9439.68154 HOMO: -6.70761 LUMO: -0.31837 factor:1 | 1 (-1.54917) | -1 | -1 |
| G: -3173.76668 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -9438.88095 HOMO: -6.57155 LUMO: 1.76874 factor:1 | 1 (-0.74859) | -1 | -1 |
| G: -3173.76668 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -9438.95818 HOMO: -6.84366 LUMO: 2.04358 factor:1 | 1 (-0.82581) | -1 | -1 |
| G: -3173.76668 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -9438.86773 HOMO: -6.60420 LUMO: 1.80139 factor:1 | 1 (-0.73536) | -1 | -1 |
| G: -3173.76668 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -9438.85823 HOMO: -7.03686 LUMO: 2.21229 factor:1 | 1 (-0.72586) | -1 | -1 |
| G: -3173.76668 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -9438.63124 HOMO: -6.77564 LUMO: 1.97555 factor:1 | 1 (-0.49887) | -1 | -1 |
| G: -3173.76668 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -9438.47341 HOMO: -6.40012 LUMO: 2.17691 factor:1 | 1 (-0.34104) | -1 | -1 |
| G: -3173.76668 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -9439.48627 HOMO: -6.80013 LUMO: 2.25582 factor:1 | 1 (-1.35390) | -1 | -1 |
| G: -3173.76668 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -9439.63378 HOMO: -6.74298 LUMO: 2.31569 factor:1 | 1 (-1.50142) | -1 | -1 |
| G: -3173.76668 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -9439.38091 HOMO: -6.68856 LUMO: 1.85854 factor:1 | 1 (-1.24854) | -1 | -1 |
| G: -3173.76668 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -9438.69216 HOMO: -6.17971 LUMO: 1.52928 factor:1 | 1 (-0.55979) | -1 | -1 |
| G: -3173.76668 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -9438.76754 HOMO: -6.54162 LUMO: 1.91840 factor:1 | 1 (-0.63517) | -1 | -1 |
| G: -3173.76668 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -9439.51642 HOMO: -6.80013 LUMO: -0.55511 factor:1 | 1 (-1.38405) | -1 | -1 |
| G: -3173.76668 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -9440.29663 HOMO: -7.46953 LUMO: 0.28572 factor:1 | 1 (-2.16426) | -1 | -1 |
| G: -3173.76668 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -9439.63455 HOMO: -6.61781 LUMO: -0.54967 factor:1 | 1 (-1.50218) | -1 | -1 |
| G: -3173.76668 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -9439.39068 HOMO: -6.56339 LUMO: -0.47892 factor:1 | 1 (-1.25831) | -1 | -1 |
| G: -3173.76668 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -9439.89967 HOMO: -6.65591 LUMO: -0.25307 factor:1 | 1 (-1.76730) | -1 | -1 |
| G: -3173.76668 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -9439.51215 HOMO: -6.62869 LUMO: -0.23402 factor:1 | 1 (-1.37978) | -1 | -1 |
| G: -3173.76668 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -9439.70900 HOMO: -6.58243 LUMO: -0.19048 factor:1 | 1 (-1.57663) | -1 | -1 |
| G: -3173.76668 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -9440.52956 HOMO: -7.27632 LUMO: 0.52790 factor:1 | 1 (-2.39719) | -1 | -1 |
| G: -3173.76668 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -9440.67440 HOMO: -7.21102 LUMO: 0.57688 factor:1 | 1 (-2.54203) | -1 | -1 |
| G: -3173.76668 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -9439.47166 HOMO: -6.72393 LUMO: -0.53879 factor:1 | 1 (-1.33929) | -1 | -1 |
| G: -3173.76668 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -9439.72826 HOMO: -7.42054 LUMO: -0.99322 factor:1 | 1 (-1.59589) | -1 | -1 |
| G: -3173.76668 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -9439.48020 HOMO: -6.88992 LUMO: -0.71838 factor:1 | 1 (-1.34783) | -1 | -1 |
| G: -3173.76668 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -9439.34464 HOMO: -6.88176 LUMO: -0.61226 factor:1 | 1 (-1.21227) | -1 | -1 |
| G: -3173.76668 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -9439.69210 HOMO: -7.36340 LUMO: -1.04492 factor:1 | 1 (-1.55973) | -1 | -1 |
| G: -3173.76668 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -9439.64557 HOMO: -6.65863 LUMO: -0.41906 factor:1 | 1 (-1.51320) | -1 | -1 |
| G: -3173.76668 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -9439.97031 HOMO: -7.15115 LUMO: -0.66396 factor:1 | 1 (-1.83794) | -1 | -1 |
| G: -3173.76668 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -9440.07504 HOMO: -7.10489 LUMO: -0.64491 factor:1 | 1 (-1.94268) | -1 | -1 |
| G: -3173.76668 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -9440.52722 HOMO: -7.20285 LUMO: 0.47892 factor:1 | 1 (-2.39485) | -1 | -1 |
| G: -3173.76668 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -9439.84859 HOMO: -6.55794 LUMO: -0.28844 factor:1 | 1 (-1.71622) | -1 | -1 |
| G: -3173.76668 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -9440.07143 HOMO: -7.19197 LUMO: -0.69661 factor:1 | 1 (-1.93906) | -1 | -1 |
| G: -3173.76668 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -9439.67150 HOMO: -6.56883 LUMO: -0.32926 factor:1 | 1 (-1.53913) | -1 | -1 |
| G: -3173.76668 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -9438.81905 HOMO: -6.70761 LUMO: 1.95650 factor:1 | 1 (-0.68668) | -1 | -1 |
| G: -3173.76668 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -9438.52103 HOMO: -6.60420 LUMO: 1.80684 factor:1 | 1 (-0.38866) | -1 | -1 |
| G: -3173.76668 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -9438.68816 HOMO: -6.84094 LUMO: 1.64085 factor:1 | 1 (-0.55579) | -1 | -1 |
| G: -3173.76668 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -9438.35833 HOMO: -6.69128 LUMO: 1.90208 factor:1 | 1 (-0.22596) | -1 | -1 |
| G: -3173.76668 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -9438.84019 HOMO: -6.75387 LUMO: 1.70343 factor:1 | 1 (-0.70782) | -1 | -1 |
| G: -3173.76668 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -9438.65464 HOMO: -7.07496 LUMO: 2.10072 factor:1 | 1 (-0.52227) | -1 | -1 |
| G: -3173.76668 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -9438.43311 HOMO: -6.99877 LUMO: 2.24494 factor:1 | 1 (-0.30074) | -1 | -1 |
| G: -3173.76668 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -9438.46827 HOMO: -6.63414 LUMO: 2.17691 factor:1 | 1 (-0.33590) | -1 | -1 |
| G: -3173.76668 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -9438.58892 HOMO: -6.44638 LUMO: 1.78235 factor:1 | 1 (-0.45655) | -1 | -1 |
| G: -3173.76668 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -9438.61358 HOMO: -6.87632 LUMO: 1.84221 factor:1 | 1 (-0.48121) | -1 | -1 |
| G: -3173.76668 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -9438.74209 HOMO: -6.85183 LUMO: 1.68711 factor:1 | 1 (-0.60973) | -1 | -1 |
| G: -3173.76668 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -9438.89249 HOMO: -6.96339 LUMO: 2.26671 factor:1 | 1 (-0.76012) | -1 | -1 |
| G: -3173.76668 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -9438.71682 HOMO: -6.63141 LUMO: 1.96738 factor:1 | 1 (-0.58445) | -1 | -1 |
| G: -3173.76668 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -9438.46759 HOMO: -6.37019 LUMO: 2.23133 factor:1 | 1 (-0.33522) | -1 | -1 |
| G: -3173.76668 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -9438.87129 HOMO: -7.11034 LUMO: 2.32385 factor:1 | 1 (-0.73893) | 1 | 1 |
| G: -3173.76668 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -9438.81622 HOMO: -6.91986 LUMO: 1.65445 factor:1 | 1 (-0.68385) | -1 | -1 |
| G: -3173.76668 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -9438.83812 HOMO: -7.12938 LUMO: 2.28304 factor:1 | 1 (-0.70575) | 1 | 1 |
| G: -3173.76668 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -9439.42260 HOMO: -6.54978 LUMO: 1.92112 factor:1 | 1 (-1.29023) | -1 | -1 |
| G: -3173.76668 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -9439.65509 HOMO: -6.83006 LUMO: 2.48712 factor:1 | 1 (-1.52272) | -1 | -1 |
| G: -3173.76668 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -9439.44083 HOMO: -6.97972 LUMO: 1.96738 factor:1 | 1 (-1.30846) | -1 | -1 |
| G: -3173.76668 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -9438.84253 HOMO: -6.69944 LUMO: 2.06262 factor:1 | 1 (-0.71016) | -1 | -1 |
| G: -3173.76668 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -9438.50889 HOMO: -6.76747 LUMO: 2.10888 factor:1 | 1 (-0.37652) | -1 | -1 |
| G: -3173.76668 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -9438.68525 HOMO: -6.91169 LUMO: 2.06534 factor:1 | 1 (-0.55288) | -1 | -1 |
| G: -3173.76668 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -9438.67241 HOMO: -7.03414 LUMO: 1.93473 factor:1 | 1 (-0.54004) | -1 | -1 |
| G: -3173.76668 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -9439.48012 HOMO: -7.03142 LUMO: 2.52250 factor:1 | 1 (-1.34775) | -1 | -1 |
| G: -3173.76668 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -9439.26183 HOMO: -6.34025 LUMO: 2.61229 factor:1 | 1 (-1.12946) | -1 | -1 |
| G: -3173.76668 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -9439.36366 HOMO: -6.98788 LUMO: 2.28304 factor:1 | 1 (-1.23129) | -1 | -1 |
| G: -3173.76668 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -9439.56595 HOMO: -6.97700 LUMO: 2.53882 factor:1 | 1 (-1.43358) | -1 | -1 |
| G: -3173.76668 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -9439.38298 HOMO: -6.58788 LUMO: 1.94289 factor:1 | 1 (-1.25061) | -1 | -1 |
| G: -3173.76668 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -9439.40828 HOMO: -6.78652 LUMO: 2.13609 factor:1 | 1 (-1.27591) | -1 | -1 |
| G: -3173.76668 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -9439.30295 HOMO: -6.55250 LUMO: 1.82861 factor:1 | 1 (-1.17058) | -1 | -1 |
| G: -3173.76668 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -9439.40600 HOMO: -6.45998 LUMO: 1.75786 factor:1 | 1 (-1.27363) | -1 | -1 |
| G: -3173.76668 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -9439.47174 HOMO: -6.78924 LUMO: 2.33746 factor:1 | 1 (-1.33937) | -1 | -1 |
| G: -3173.76668 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -9439.54434 HOMO: -6.85727 LUMO: 1.76058 factor:1 | 1 (-1.41197) | -1 | -1 |
| G: -3173.76668 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -9438.78231 HOMO: -6.70489 LUMO: 1.84493 factor:1 | 1 (-0.64994) | -1 | -1 |
| G: -3173.76668 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -9438.89987 HOMO: -6.71305 LUMO: 1.53472 factor:1 | 1 (-0.76750) | -1 | -1 |
| G: -3173.76668 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -9438.92613 HOMO: -6.76747 LUMO: 1.48846 factor:1 | 1 (-0.79376) | -1 | -1 |
| G: -3173.76668 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -9438.41387 HOMO: -6.69128 LUMO: 1.95922 factor:1 | 1 (-0.28150) | -1 | -1 |
| G: -3173.76668 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -9438.32919 HOMO: -6.67495 LUMO: 2.05446 factor:1 | 1 (-0.19682) | -1 | -1 |
| G: -3173.76668 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -9438.23311 HOMO: -6.63686 LUMO: 2.25310 factor:1 | 1 (-0.10074) | -1 | -1 |
| G: -3173.76668 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -9438.56971 HOMO: -6.63958 LUMO: 2.14154 factor:1 | 1 (-0.43734) | -1 | -1 |
| G: -3173.76668 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -9438.41716 HOMO: -6.62597 LUMO: 2.01908 factor:1 | 1 (-0.28479) | -1 | -1 |
| G: -3173.76668 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -9438.65951 HOMO: -7.07768 LUMO: 2.14154 factor:1 | 1 (-0.52714) | -1 | -1 |
| G: -3173.76668 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -9438.42405 HOMO: -6.19603 LUMO: 2.01092 factor:1 | 1 (-0.29168) | -1 | -1 |
| G: -3173.76668 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -9438.29602 HOMO: -6.65046 LUMO: 2.15786 factor:1 | 1 (-0.16365) | -1 | -1 |
| G: -3173.76668 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -9438.38990 HOMO: -6.92258 LUMO: 2.31841 factor:1 | 1 (-0.25753) | -1 | -1 |
| G: -3173.76668 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -9438.50263 HOMO: -6.90081 LUMO: 2.19324 factor:1 | 1 (-0.37027) | -1 | -1 |
| G: -3173.76668 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -9438.81127 HOMO: -6.85455 LUMO: 1.95650 factor:1 | 1 (-0.67890) | -1 | -1 |
| G: -3173.76668 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -9438.58239 HOMO: -6.57699 LUMO: 1.76058 factor:1 | 1 (-0.45002) | -1 | -1 |
| G: -3173.76668 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -9438.58375 HOMO: -6.90625 LUMO: 1.97555 factor:1 | 1 (-0.45138) | -1 | -1 |
| G: -3173.76668 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -9438.78544 HOMO: -6.97428 LUMO: 1.92929 factor:1 | 1 (-0.65307) | -1 | -1 |
| G: -3173.76668 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -9439.49463 HOMO: -6.61781 LUMO: -0.41906 factor:1 | 1 (-1.36226) | -1 | -1 |
| G: -3173.76668 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -9439.33797 HOMO: -6.62869 LUMO: -0.81906 factor:1 | 1 (-1.20560) | -1 | -1 |
| G: -3173.76668 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -9438.66666 HOMO: -7.01237 LUMO: 2.00548 factor:1 | 1 (-0.53430) | -1 | -1 |
| G: -3173.76668 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -9438.37686 HOMO: -6.85727 LUMO: 2.17691 factor:1 | 1 (-0.24449) | -1 | -1 |
| G: -3173.76668 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -9438.62304 HOMO: -6.71849 LUMO: 1.58914 factor:1 | 1 (-0.49068) | -1 | -1 |
| G: -3173.76668 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -9440.14680 HOMO: -7.52395 LUMO: 0.27211 factor:1 | 1 (-2.01443) | -1 | -1 |
| G: -3173.76668 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -9439.36344 HOMO: -6.96611 LUMO: -0.72654 factor:1 | 1 (-1.23107) | -1 | -1 |
| G: -3173.76668 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -9439.40894 HOMO: -6.89537 LUMO: -0.68028 factor:1 | 1 (-1.27657) | -1 | -1 |
| G: -3173.76668 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -9439.29122 HOMO: -6.84911 LUMO: -0.58504 factor:1 | 1 (-1.15885) | -1 | -1 |
| G: -3173.76668 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -9439.48733 HOMO: -6.79196 LUMO: -0.55783 factor:1 | 1 (-1.35496) | -1 | -1 |
| G: -3173.76668 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -9438.62400 HOMO: -6.67767 LUMO: 1.79323 factor:1 | 1 (-0.49163) | -1 | -1 |
| G: -3173.76668 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -9438.57997 HOMO: -6.54434 LUMO: 1.91024 factor:1 | 1 (-0.44760) | -1 | -1 |
| G: -3173.76668 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -9438.69916 HOMO: -6.62869 LUMO: 1.69799 factor:1 | 1 (-0.56679) | -1 | -1 |
| G: -3173.76668 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -9438.57396 HOMO: -6.72393 LUMO: 2.12249 factor:1 | 1 (-0.44159) | -1 | -1 |
| G: -3173.76668 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -9438.46111 HOMO: -6.66407 LUMO: 2.05990 factor:1 | 1 (-0.32874) | -1 | -1 |
| G: -3173.76668 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -9438.61817 HOMO: -7.00149 LUMO: 1.82044 factor:1 | 1 (-0.48580) | -1 | -1 |
| G: -3173.76668 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -9438.66628 HOMO: -7.12122 LUMO: 2.16058 factor:1 | 1 (-0.53391) | 1 | 1 |
| G: -3173.76668 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -9438.25547 HOMO: -6.63141 LUMO: 2.21229 factor:1 | 1 (-0.12310) | -1 | -1 |
| G: -3173.76668 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -9437.93158 HOMO: -6.37835 LUMO: 2.32113 factor:1 | -1 (0.20079) | -1 | -1 |
| G: -3173.76668 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -9438.39221 HOMO: -6.99605 LUMO: 2.00548 factor:1 | 1 (-0.25984) | -1 | -1 |
| G: -3173.76668 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -9439.35732 HOMO: -6.85999 LUMO: 2.39460 factor:1 | 1 (-1.22495) | -1 | -1 |
| G: -3173.76668 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -9439.46894 HOMO: -6.85727 LUMO: 2.48712 factor:1 | 1 (-1.33657) | -1 | -1 |
| G: -3173.76668 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -9439.40888 HOMO: -7.04231 LUMO: 2.40277 factor:1 | 1 (-1.27651) | -1 | -1 |
| G: -3173.76668 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -9439.01649 HOMO: -6.60692 LUMO: 2.26671 factor:1 | 1 (-0.88413) | -1 | -1 |
| G: -3173.76668 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -9439.37775 HOMO: -6.67495 LUMO: 2.14698 factor:1 | 1 (-1.24538) | -1 | -1 |
| G: -3173.76668 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -9439.19429 HOMO: -6.73210 LUMO: 2.06807 factor:1 | 1 (-1.06192) | -1 | -1 |
| G: -3173.76668 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -9438.52519 HOMO: -7.20013 LUMO: 2.02181 factor:1 | 1 (-0.39282) | 1 | 1 |
| G: -3173.76668 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -9438.71094 HOMO: -7.18653 LUMO: 2.29936 factor:1 | 1 (-0.57857) | 1 | 1 |
| G: -3173.76668 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -9438.33349 HOMO: -6.92802 LUMO: 2.36195 factor:1 | 1 (-0.20112) | -1 | -1 |
| G: -3173.76668 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -9438.66266 HOMO: -6.89537 LUMO: 1.78779 factor:1 | 1 (-0.53030) | -1 | -1 |
| G: -3173.76668 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -9438.37719 HOMO: -6.96067 LUMO: 2.31297 factor:1 | 1 (-0.24482) | -1 | -1 |
| G: -3173.76668 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -9438.29330 HOMO: -6.91441 LUMO: 2.50345 factor:1 | 1 (-0.16093) | -1 | -1 |
| G: -3173.76668 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -9438.49042 HOMO: -7.17292 LUMO: 2.12521 factor:1 | 1 (-0.35805) | 1 | 1 |
| G: -3173.76668 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -9438.40873 HOMO: -6.93618 LUMO: 2.35106 factor:1 | 1 (-0.27636) | -1 | -1 |
| G: -3173.76668 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -9438.58609 HOMO: -6.75931 LUMO: 1.61908 factor:1 | 1 (-0.45372) | -1 | -1 |
| G: -3173.76668 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -9438.62068 HOMO: -6.35930 LUMO: 1.23540 factor:1 | 1 (-0.48831) | -1 | -1 |
| G: -3173.76668 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -9438.32775 HOMO: -6.17971 LUMO: 1.84493 factor:1 | 1 (-0.19538) | -1 | -1 |
| G: -3173.76668 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -9439.24861 HOMO: -6.72665 LUMO: 2.61229 factor:1 | 1 (-1.11624) | -1 | -1 |
| G: -3173.76668 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -9438.91089 HOMO: -6.62869 LUMO: 2.28304 factor:1 | 1 (-0.77852) | -1 | -1 |
| G: -3612.09786 HOMO: -8.88180 LUMO: 1.02315 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -9875.15025 HOMO: -6.58243 LUMO: 0.28028 factor:1 | -1 (1.31330) | -1 | -1 |
| G: -3612.09786 HOMO: -8.88180 LUMO: 1.02315 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -9874.91131 HOMO: -6.79468 LUMO: 0.14966 factor:1 | -1 (1.55225) | -1 | -1 |
| G: -3612.09786 HOMO: -8.88180 LUMO: 1.02315 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -9875.23523 HOMO: -6.63141 LUMO: 0.31021 factor:1 | -1 (1.22832) | -1 | -1 |
| G: -3612.09786 HOMO: -8.88180 LUMO: 1.02315 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -9875.16146 HOMO: -6.81101 LUMO: 0.13878 factor:1 | -1 (1.30209) | -1 | -1 |
| G: -3612.09786 HOMO: -8.88180 LUMO: 1.02315 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -9877.43783 HOMO: -6.72665 LUMO: 0.65579 factor:1 | 1 (-0.97428) | -1 | -1 |
| G: -3612.09786 HOMO: -8.88180 LUMO: 1.02315 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -9877.16112 HOMO: -6.53073 LUMO: 0.91430 factor:1 | 1 (-0.69756) | -1 | -1 |
| G: -3612.09786 HOMO: -8.88180 LUMO: 1.02315 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -9877.87903 HOMO: -7.19197 LUMO: 1.62996 factor:1 | 1 (-1.41548) | 1 | 1 |
| G: -3612.09786 HOMO: -8.88180 LUMO: 1.02315 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -9877.43462 HOMO: -6.69400 LUMO: 0.84627 factor:1 | 1 (-0.97107) | -1 | -1 |
| G: -3612.09786 HOMO: -8.88180 LUMO: 1.02315 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -9877.48561 HOMO: -6.76475 LUMO: 0.51974 factor:1 | 1 (-1.02206) | -1 | -1 |
| G: -3612.09786 HOMO: -8.88180 LUMO: 1.02315 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -9876.90552 HOMO: -6.67767 LUMO: 0.52246 factor:1 | 1 (-0.44197) | -1 | -1 |
| G: -3612.09786 HOMO: -8.88180 LUMO: 1.02315 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -9877.05954 HOMO: -6.73210 LUMO: 0.94424 factor:1 | 1 (-0.59598) | -1 | -1 |
| G: -3612.09786 HOMO: -8.88180 LUMO: 1.02315 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -9876.10395 HOMO: -6.97972 LUMO: 0.60409 factor:1 | -1 (0.35960) | -1 | -1 |
| G: -3612.09786 HOMO: -8.88180 LUMO: 1.02315 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -9876.38048 HOMO: -7.38517 LUMO: 0.73743 factor:1 | -1 (0.08308) | -1 | -1 |
| G: -3612.09786 HOMO: -8.88180 LUMO: 1.02315 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -9877.19872 HOMO: -6.48992 LUMO: 1.08301 factor:1 | 1 (-0.73517) | -1 | -1 |
| G: -3612.09786 HOMO: -8.88180 LUMO: 1.02315 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -9877.75386 HOMO: -7.18381 LUMO: 1.61908 factor:1 | 1 (-1.29031) | 1 | 1 |
| G: -3612.09786 HOMO: -8.88180 LUMO: 1.02315 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -9877.15235 HOMO: -6.74842 LUMO: 0.57960 factor:1 | 1 (-0.68880) | -1 | -1 |
| G: -3612.09786 HOMO: -8.88180 LUMO: 1.02315 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -9876.91042 HOMO: -6.67495 LUMO: 0.77280 factor:1 | 1 (-0.44687) | -1 | -1 |
| G: -3612.09786 HOMO: -8.88180 LUMO: 1.02315 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -9877.15586 HOMO: -6.74570 LUMO: 0.77280 factor:1 | 1 (-0.69231) | -1 | -1 |
| G: -3612.09786 HOMO: -8.88180 LUMO: 1.02315 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -9877.02076 HOMO: -6.73754 LUMO: 0.86804 factor:1 | 1 (-0.55721) | -1 | -1 |
| G: -3612.09786 HOMO: -8.88180 LUMO: 1.02315 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -9877.17750 HOMO: -6.66135 LUMO: 0.94424 factor:1 | 1 (-0.71395) | -1 | -1 |
| G: -3612.09786 HOMO: -8.88180 LUMO: 1.02315 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -9877.30262 HOMO: -6.44638 LUMO: 1.00138 factor:1 | 1 (-0.83906) | -1 | -1 |
| G: -3612.09786 HOMO: -8.88180 LUMO: 1.02315 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -9876.98163 HOMO: -6.65591 LUMO: 1.02043 factor:1 | 1 (-0.51808) | -1 | -1 |
| G: -3612.09786 HOMO: -8.88180 LUMO: 1.02315 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -9876.15732 HOMO: -7.17564 LUMO: 0.50069 factor:1 | -1 (0.30624) | -1 | -1 |
| G: -3612.09786 HOMO: -8.88180 LUMO: 1.02315 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -9876.93815 HOMO: -6.59332 LUMO: 0.79457 factor:1 | 1 (-0.47459) | -1 | -1 |
| G: -3612.09786 HOMO: -8.88180 LUMO: 1.02315 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -9877.59606 HOMO: -6.76747 LUMO: 1.73881 factor:1 | 1 (-1.13251) | -1 | -1 |
| G: -3612.09786 HOMO: -8.88180 LUMO: 1.02315 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -9876.43174 HOMO: -7.00421 LUMO: 1.07485 factor:1 | -1 (0.03181) | -1 | -1 |
| G: -3612.09786 HOMO: -8.88180 LUMO: 1.02315 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -9876.53392 HOMO: -6.94979 LUMO: 1.67894 factor:1 | 1 (-0.07037) | -1 | -1 |
| G: -3612.09786 HOMO: -8.88180 LUMO: 1.02315 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -9877.20270 HOMO: -6.66135 LUMO: 0.47076 factor:1 | 1 (-0.73914) | -1 | -1 |
| G: -3612.09786 HOMO: -8.88180 LUMO: 1.02315 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -9877.64994 HOMO: -6.74298 LUMO: 1.85037 factor:1 | 1 (-1.18639) | -1 | -1 |
| G: -3612.09786 HOMO: -8.88180 LUMO: 1.02315 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -9877.07181 HOMO: -6.65318 LUMO: 0.95240 factor:1 | 1 (-0.60826) | -1 | -1 |
| G: -3612.09786 HOMO: -8.88180 LUMO: 1.02315 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -9876.65090 HOMO: -6.63958 LUMO: 0.78097 factor:1 | 1 (-0.18735) | -1 | -1 |
| G: -3612.09786 HOMO: -8.88180 LUMO: 1.02315 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -9876.81983 HOMO: -6.11712 LUMO: 0.40001 factor:1 | 1 (-0.35628) | -1 | -1 |
| G: -3612.09786 HOMO: -8.88180 LUMO: 1.02315 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -9876.24382 HOMO: -7.08312 LUMO: 0.92519 factor:1 | -1 (0.21973) | -1 | -1 |
| G: -3612.09786 HOMO: -8.88180 LUMO: 1.02315 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -9875.85731 HOMO: -6.96067 LUMO: 0.54695 factor:1 | -1 (0.60624) | -1 | -1 |
| G: -3612.09786 HOMO: -8.88180 LUMO: 1.02315 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -9876.74334 HOMO: -6.74026 LUMO: 0.60137 factor:1 | 1 (-0.27979) | -1 | -1 |
| G: -3612.09786 HOMO: -8.88180 LUMO: 1.02315 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -9876.95107 HOMO: -6.74298 LUMO: 0.59593 factor:1 | 1 (-0.48752) | -1 | -1 |
| G: -3612.09786 HOMO: -8.88180 LUMO: 1.02315 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -9877.28419 HOMO: -6.93074 LUMO: 0.60681 factor:1 | 1 (-0.82064) | -1 | -1 |
| G: -3612.09786 HOMO: -8.88180 LUMO: 1.02315 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -9877.04754 HOMO: -6.41644 LUMO: 0.35919 factor:1 | 1 (-0.58398) | -1 | -1 |
| G: -3612.09786 HOMO: -8.88180 LUMO: 1.02315 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -9877.37059 HOMO: -6.41917 LUMO: 1.73064 factor:1 | 1 (-0.90704) | -1 | -1 |
| G: -3612.09786 HOMO: -8.88180 LUMO: 1.02315 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -9875.28154 HOMO: -4.64226 LUMO: -0.87893 factor:1 | -1 (1.18201) | -1 | -1 |
| G: -3612.09786 HOMO: -8.88180 LUMO: 1.02315 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -9877.20822 HOMO: -6.59604 LUMO: 0.90342 factor:1 | 1 (-0.74467) | -1 | -1 |
| G: -3612.09786 HOMO: -8.88180 LUMO: 1.02315 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -9877.35598 HOMO: -6.79468 LUMO: 0.50069 factor:1 | 1 (-0.89242) | -1 | -1 |
| G: -3612.09786 HOMO: -8.88180 LUMO: 1.02315 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -9877.40526 HOMO: -7.04503 LUMO: 0.52518 factor:1 | 1 (-0.94170) | -1 | -1 |
| G: -3612.09786 HOMO: -8.88180 LUMO: 1.02315 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -9877.14593 HOMO: -6.69400 LUMO: 0.54423 factor:1 | 1 (-0.68238) | -1 | -1 |
| G: -3612.09786 HOMO: -8.88180 LUMO: 1.02315 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -9877.08560 HOMO: -6.51713 LUMO: 0.95240 factor:1 | 1 (-0.62205) | -1 | -1 |
| G: -3612.09786 HOMO: -8.88180 LUMO: 1.02315 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -9875.21270 HOMO: -6.88176 LUMO: 1.79323 factor:1 | -1 (1.25085) | -1 | -1 |
| G: -3612.09786 HOMO: -8.88180 LUMO: 1.02315 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -9875.91636 HOMO: -6.71849 LUMO: 0.28844 factor:1 | -1 (0.54719) | -1 | -1 |
| G: -3612.09786 HOMO: -8.88180 LUMO: 1.02315 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -9875.93296 HOMO: -6.94979 LUMO: 0.51974 factor:1 | -1 (0.53059) | -1 | -1 |
| G: -3612.09786 HOMO: -8.88180 LUMO: 1.02315 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -9876.69863 HOMO: -6.76203 LUMO: 0.94151 factor:1 | 1 (-0.23508) | -1 | -1 |
| G: -3612.09786 HOMO: -8.88180 LUMO: 1.02315 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -9875.76531 HOMO: -6.91169 LUMO: 0.89525 factor:1 | -1 (0.69824) | -1 | -1 |
| G: -3612.09786 HOMO: -8.88180 LUMO: 1.02315 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -9876.82620 HOMO: -6.83006 LUMO: 0.89253 factor:1 | 1 (-0.36265) | -1 | -1 |
| G: -3612.09786 HOMO: -8.88180 LUMO: 1.02315 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -9875.95247 HOMO: -7.08857 LUMO: 0.60409 factor:1 | -1 (0.51108) | -1 | -1 |
| G: -3612.09786 HOMO: -8.88180 LUMO: 1.02315 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -9875.09232 HOMO: -6.91713 LUMO: 1.76330 factor:1 | -1 (1.37124) | -1 | -1 |
| G: -3612.09786 HOMO: -8.88180 LUMO: 1.02315 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -9875.16364 HOMO: -6.47359 LUMO: 1.56193 factor:1 | -1 (1.29992) | -1 | -1 |
| G: -4185.45180 HOMO: -6.91169 LUMO: -0.53879 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10449.61058 HOMO: -7.00149 LUMO: 1.47214 factor:1 | -1 (0.20692) | -1 | -1 |
| G: -4185.45180 HOMO: -6.91169 LUMO: -0.53879 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10449.28892 HOMO: -7.03686 LUMO: 1.97283 factor:1 | -1 (0.52858) | -1 | -1 |
| G: -4185.45180 HOMO: -6.91169 LUMO: -0.53879 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10449.43934 HOMO: -7.00965 LUMO: 1.64629 factor:1 | -1 (0.37816) | -1 | -1 |
| G: -4185.45180 HOMO: -6.91169 LUMO: -0.53879 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10449.59042 HOMO: -7.06952 LUMO: 1.67622 factor:1 | -1 (0.22708) | 1 | -1 |
| G: -4185.45180 HOMO: -6.91169 LUMO: -0.53879 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10449.18396 HOMO: -6.80557 LUMO: 1.70615 factor:1 | -1 (0.63354) | -1 | -1 |
| G: -4185.45180 HOMO: -6.91169 LUMO: -0.53879 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10449.33637 HOMO: -6.80829 LUMO: 1.71704 factor:1 | -1 (0.48112) | -1 | -1 |
| G: -4185.45180 HOMO: -6.91169 LUMO: -0.53879 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10449.27354 HOMO: -7.26544 LUMO: 1.89935 factor:1 | -1 (0.54396) | 1 | -1 |
| G: -4184.20345 HOMO: -7.29809 LUMO: 2.83543 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10449.61058 HOMO: -7.00149 LUMO: 1.47214 factor:1 | 1 (-1.04143) | -1 | -1 |
| G: -4184.20345 HOMO: -7.29809 LUMO: 2.83543 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10449.28892 HOMO: -7.03686 LUMO: 1.97283 factor:1 | 1 (-0.71977) | -1 | -1 |
| G: -4184.20345 HOMO: -7.29809 LUMO: 2.83543 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10449.43934 HOMO: -7.00965 LUMO: 1.64629 factor:1 | 1 (-0.87019) | -1 | -1 |
| G: -4184.20345 HOMO: -7.29809 LUMO: 2.83543 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10449.59042 HOMO: -7.06952 LUMO: 1.67622 factor:1 | 1 (-1.02127) | -1 | -1 |
| G: -4184.20345 HOMO: -7.29809 LUMO: 2.83543 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10449.18396 HOMO: -6.80557 LUMO: 1.70615 factor:1 | 1 (-0.61481) | -1 | -1 |
| G: -4184.20345 HOMO: -7.29809 LUMO: 2.83543 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10449.33637 HOMO: -6.80829 LUMO: 1.71704 factor:1 | 1 (-0.76723) | -1 | -1 |
| G: -4184.20345 HOMO: -7.29809 LUMO: 2.83543 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10449.27354 HOMO: -7.26544 LUMO: 1.89935 factor:1 | 1 (-0.70439) | -1 | -1 |
| G: -3206.83700 HOMO: -7.85865 LUMO: 2.83543 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -9471.98959 HOMO: -7.00149 LUMO: 1.75241 factor:1 | 1 (-0.78690) | -1 | -1 |
| G: -3206.83700 HOMO: -7.85865 LUMO: 2.83543 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -9471.84235 HOMO: -6.91169 LUMO: 2.07079 factor:1 | 1 (-0.63966) | -1 | -1 |
| G: -3206.83700 HOMO: -7.85865 LUMO: 2.83543 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -9472.13297 HOMO: -7.11034 LUMO: 1.76330 factor:1 | 1 (-0.93028) | -1 | -1 |
| G: -3206.83700 HOMO: -7.85865 LUMO: 2.83543 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -9472.10478 HOMO: -6.87360 LUMO: 2.02725 factor:1 | 1 (-0.90208) | -1 | -1 |
| G: -3206.83700 HOMO: -7.85865 LUMO: 2.83543 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -9471.79068 HOMO: -7.08584 LUMO: 1.82044 factor:1 | 1 (-0.58798) | -1 | -1 |
| G: -3206.83700 HOMO: -7.85865 LUMO: 2.83543 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -9472.06154 HOMO: -6.90625 LUMO: 1.68166 factor:1 | 1 (-0.85885) | -1 | -1 |
| G: -3206.83700 HOMO: -7.85865 LUMO: 2.83543 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -9471.68297 HOMO: -6.71577 LUMO: 1.93201 factor:1 | 1 (-0.48028) | -1 | -1 |
| G: -3206.83700 HOMO: -7.85865 LUMO: 2.83543 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -9471.88279 HOMO: -6.99605 LUMO: 2.08439 factor:1 | 1 (-0.68009) | -1 | -1 |
| G: -3206.83700 HOMO: -7.85865 LUMO: 2.83543 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -9471.92412 HOMO: -7.02326 LUMO: 1.97010 factor:1 | 1 (-0.72143) | -1 | -1 |
| G: -3206.83700 HOMO: -7.85865 LUMO: 2.83543 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -9471.92551 HOMO: -6.99877 LUMO: 2.15514 factor:1 | 1 (-0.72282) | -1 | -1 |
| G: -3206.83700 HOMO: -7.85865 LUMO: 2.83543 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -9471.73851 HOMO: -6.75387 LUMO: 1.95106 factor:1 | 1 (-0.53582) | -1 | -1 |
| G: -3206.83700 HOMO: -7.85865 LUMO: 2.83543 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -9471.76502 HOMO: -7.10761 LUMO: 2.06262 factor:1 | 1 (-0.56232) | -1 | -1 |
| G: -3206.83700 HOMO: -7.85865 LUMO: 2.83543 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -9471.93427 HOMO: -7.03142 LUMO: 1.91568 factor:1 | 1 (-0.73158) | -1 | -1 |
| G: -3206.83700 HOMO: -7.85865 LUMO: 2.83543 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -9471.71740 HOMO: -6.98788 LUMO: 1.98371 factor:1 | 1 (-0.51470) | -1 | -1 |
| G: -3206.83700 HOMO: -7.85865 LUMO: 2.83543 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -9472.01098 HOMO: -6.94707 LUMO: 1.68438 factor:1 | 1 (-0.80829) | -1 | -1 |
| G: -3206.83700 HOMO: -7.85865 LUMO: 2.83543 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -9471.87911 HOMO: -6.88176 LUMO: 2.20684 factor:1 | 1 (-0.67642) | -1 | -1 |
| G: -3206.83700 HOMO: -7.85865 LUMO: 2.83543 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -9471.67438 HOMO: -6.73210 LUMO: 2.18780 factor:1 | 1 (-0.47168) | -1 | -1 |
| G: -3206.83700 HOMO: -7.85865 LUMO: 2.83543 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -9471.58833 HOMO: -6.83822 LUMO: 2.06807 factor:1 | 1 (-0.38564) | -1 | -1 |
| G: -3206.83700 HOMO: -7.85865 LUMO: 2.83543 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -9471.44945 HOMO: -6.78924 LUMO: 2.42181 factor:1 | 1 (-0.24675) | -1 | -1 |
| G: -3206.83700 HOMO: -7.85865 LUMO: 2.83543 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -9471.98053 HOMO: -6.94707 LUMO: 1.71704 factor:1 | 1 (-0.77784) | -1 | -1 |
| G: -3206.83700 HOMO: -7.85865 LUMO: 2.83543 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -9471.88613 HOMO: -6.85183 LUMO: 1.78779 factor:1 | 1 (-0.68344) | -1 | -1 |
| G: -3206.83700 HOMO: -7.85865 LUMO: 2.83543 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -9472.14219 HOMO: -6.98788 LUMO: 1.69799 factor:1 | 1 (-0.93950) | -1 | -1 |
| G: -3206.83700 HOMO: -7.85865 LUMO: 2.83543 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -9471.80151 HOMO: -6.79468 LUMO: 2.04358 factor:1 | 1 (-0.59881) | -1 | -1 |
| G: -3206.83700 HOMO: -7.85865 LUMO: 2.83543 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -9471.77917 HOMO: -6.90081 LUMO: 1.97283 factor:1 | 1 (-0.57647) | -1 | -1 |
| G: -3206.83700 HOMO: -7.85865 LUMO: 2.83543 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -9471.72009 HOMO: -6.79468 LUMO: 2.00820 factor:1 | 1 (-0.51740) | -1 | -1 |
| G: -3206.83700 HOMO: -7.85865 LUMO: 2.83543 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -9471.79299 HOMO: -7.06408 LUMO: 2.29936 factor:1 | 1 (-0.59030) | -1 | -1 |
| G: -3206.83700 HOMO: -7.85865 LUMO: 2.83543 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -9471.69323 HOMO: -6.78924 LUMO: 2.13337 factor:1 | 1 (-0.49054) | -1 | -1 |
| G: -3206.83700 HOMO: -7.85865 LUMO: 2.83543 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -9471.48332 HOMO: -6.79468 LUMO: 2.35106 factor:1 | 1 (-0.28063) | -1 | -1 |
| G: -3206.83700 HOMO: -7.85865 LUMO: 2.83543 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -9471.57048 HOMO: -6.82734 LUMO: 2.16603 factor:1 | 1 (-0.36779) | -1 | -1 |
| G: -3206.83700 HOMO: -7.85865 LUMO: 2.83543 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -9471.35353 HOMO: -6.79740 LUMO: 2.36739 factor:1 | 1 (-0.15083) | -1 | -1 |
| G: -3206.83700 HOMO: -7.85865 LUMO: 2.83543 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -9471.75786 HOMO: -7.14027 LUMO: 2.10888 factor:1 | 1 (-0.55517) | -1 | -1 |
| G: -5254.96698 HOMO: -6.61509 LUMO: -0.23674 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11518.89160 HOMO: -6.96067 LUMO: 1.59731 factor:1 | -1 (0.44107) | -1 | -1 |
| G: -5254.96698 HOMO: -6.61509 LUMO: -0.23674 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11518.65927 HOMO: -6.91169 LUMO: 1.37145 factor:1 | -1 (0.67340) | -1 | -1 |
| G: -5254.96698 HOMO: -6.61509 LUMO: -0.23674 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11518.49086 HOMO: -6.94707 LUMO: 1.73064 factor:1 | -1 (0.84181) | -1 | -1 |
| G: -5254.96698 HOMO: -6.61509 LUMO: -0.23674 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11518.83960 HOMO: -7.02326 LUMO: 1.41227 factor:1 | -1 (0.49307) | -1 | -1 |
| G: -5254.96698 HOMO: -6.61509 LUMO: -0.23674 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11518.87878 HOMO: -6.72121 LUMO: 1.43132 factor:1 | -1 (0.45389) | -1 | -1 |
| G: -5254.96698 HOMO: -6.61509 LUMO: -0.23674 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11518.53475 HOMO: -6.51168 LUMO: 1.72520 factor:1 | -1 (0.79792) | -1 | -1 |
| G: -5254.96698 HOMO: -6.61509 LUMO: -0.23674 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11518.29701 HOMO: -6.98516 LUMO: 1.92929 factor:1 | -1 (1.03567) | -1 | -1 |
| G: -5254.96698 HOMO: -6.61509 LUMO: -0.23674 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11518.16348 HOMO: -6.92802 LUMO: 2.07895 factor:1 | -1 (1.16919) | -1 | -1 |
| G: -5254.96698 HOMO: -6.61509 LUMO: -0.23674 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11518.51837 HOMO: -7.02326 LUMO: 1.86398 factor:1 | -1 (0.81430) | -1 | -1 |
| G: -5254.96698 HOMO: -6.61509 LUMO: -0.23674 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11518.65704 HOMO: -6.82462 LUMO: 1.86670 factor:1 | -1 (0.67563) | -1 | -1 |
| G: -5254.96698 HOMO: -6.61509 LUMO: -0.23674 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11518.53709 HOMO: -6.83278 LUMO: 1.71160 factor:1 | -1 (0.79558) | -1 | -1 |
| G: -5254.96698 HOMO: -6.61509 LUMO: -0.23674 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11518.89767 HOMO: -6.62869 LUMO: 1.69527 factor:1 | -1 (0.43500) | -1 | -1 |
| G: -5254.96698 HOMO: -6.61509 LUMO: -0.23674 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11518.43940 HOMO: -6.84094 LUMO: 1.27349 factor:1 | -1 (0.89327) | -1 | -1 |
| G: -5254.96698 HOMO: -6.61509 LUMO: -0.23674 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11518.70839 HOMO: -7.07768 LUMO: 1.27621 factor:1 | -1 (0.62428) | 1 | -1 |
| G: -5254.96698 HOMO: -6.61509 LUMO: -0.23674 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11518.34005 HOMO: -7.06135 LUMO: 1.55105 factor:1 | -1 (0.99262) | 1 | -1 |
| G: -5254.96698 HOMO: -6.61509 LUMO: -0.23674 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11518.55614 HOMO: -6.94162 LUMO: 1.64629 factor:1 | -1 (0.77653) | -1 | -1 |
| G: -5254.96698 HOMO: -6.61509 LUMO: -0.23674 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11518.74558 HOMO: -7.07224 LUMO: 1.65445 factor:1 | -1 (0.58709) | 1 | -1 |
| G: -5254.96698 HOMO: -6.61509 LUMO: -0.23674 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11518.53361 HOMO: -6.68584 LUMO: 1.91296 factor:1 | -1 (0.79906) | -1 | -1 |
| G: -5254.96698 HOMO: -6.61509 LUMO: -0.23674 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11518.49701 HOMO: -7.09129 LUMO: 1.73609 factor:1 | -1 (0.83566) | 1 | -1 |
| G: -5254.96698 HOMO: -6.61509 LUMO: -0.23674 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11518.59464 HOMO: -7.01237 LUMO: 2.01092 factor:1 | -1 (0.73803) | -1 | -1 |
| G: -5254.96698 HOMO: -6.61509 LUMO: -0.23674 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11518.39883 HOMO: -6.93618 LUMO: 1.63540 factor:1 | -1 (0.93384) | -1 | -1 |
| G: -5254.96698 HOMO: -6.61509 LUMO: -0.23674 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11518.58882 HOMO: -6.98516 LUMO: 1.64629 factor:1 | -1 (0.74385) | -1 | -1 |
| G: -5254.96698 HOMO: -6.61509 LUMO: -0.23674 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11518.52174 HOMO: -6.80285 LUMO: 1.95106 factor:1 | -1 (0.81093) | -1 | -1 |
| G: -5254.96698 HOMO: -6.61509 LUMO: -0.23674 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11518.31407 HOMO: -6.76747 LUMO: 1.88303 factor:1 | -1 (1.01860) | -1 | -1 |
| G: -5254.96698 HOMO: -6.61509 LUMO: -0.23674 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11518.24770 HOMO: -6.64230 LUMO: 1.90480 factor:1 | -1 (1.08497) | -1 | -1 |
| G: -5254.96698 HOMO: -6.61509 LUMO: -0.23674 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11518.10878 HOMO: -6.93618 LUMO: 2.19324 factor:1 | -1 (1.22389) | -1 | -1 |
| G: -5254.96698 HOMO: -6.61509 LUMO: -0.23674 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11518.37622 HOMO: -6.95523 LUMO: 1.80684 factor:1 | -1 (0.95645) | -1 | -1 |
| G: -5254.96698 HOMO: -6.61509 LUMO: -0.23674 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11518.54457 HOMO: -6.66135 LUMO: 1.72792 factor:1 | -1 (0.78810) | -1 | -1 |
| G: -5254.96698 HOMO: -6.61509 LUMO: -0.23674 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11518.36506 HOMO: -6.36202 LUMO: 1.89391 factor:1 | -1 (0.96761) | -1 | -1 |
| G: -5254.96698 HOMO: -6.61509 LUMO: -0.23674 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11518.12702 HOMO: -7.03959 LUMO: 2.06262 factor:1 | -1 (1.20565) | -1 | -1 |
| G: -5254.96698 HOMO: -6.61509 LUMO: -0.23674 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11518.34465 HOMO: -7.08584 LUMO: 2.01092 factor:1 | -1 (0.98802) | 1 | -1 |
| G: -5254.59478 HOMO: -6.80285 LUMO: -0.55783 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11518.89160 HOMO: -6.96067 LUMO: 1.59731 factor:1 | -1 (0.06887) | -1 | -1 |
| G: -5254.59478 HOMO: -6.80285 LUMO: -0.55783 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11518.65927 HOMO: -6.91169 LUMO: 1.37145 factor:1 | -1 (0.30120) | -1 | -1 |
| G: -5254.59478 HOMO: -6.80285 LUMO: -0.55783 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11518.49086 HOMO: -6.94707 LUMO: 1.73064 factor:1 | -1 (0.46961) | -1 | -1 |
| G: -5254.59478 HOMO: -6.80285 LUMO: -0.55783 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11518.83960 HOMO: -7.02326 LUMO: 1.41227 factor:1 | -1 (0.12087) | -1 | -1 |
| G: -5254.59478 HOMO: -6.80285 LUMO: -0.55783 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11518.87878 HOMO: -6.72121 LUMO: 1.43132 factor:1 | -1 (0.08169) | -1 | -1 |
| G: -5254.59478 HOMO: -6.80285 LUMO: -0.55783 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11518.53475 HOMO: -6.51168 LUMO: 1.72520 factor:1 | -1 (0.42572) | -1 | -1 |
| G: -5254.59478 HOMO: -6.80285 LUMO: -0.55783 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11518.29701 HOMO: -6.98516 LUMO: 1.92929 factor:1 | -1 (0.66347) | -1 | -1 |
| G: -5254.59478 HOMO: -6.80285 LUMO: -0.55783 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11518.16348 HOMO: -6.92802 LUMO: 2.07895 factor:1 | -1 (0.79699) | -1 | -1 |
| G: -5254.59478 HOMO: -6.80285 LUMO: -0.55783 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11518.51837 HOMO: -7.02326 LUMO: 1.86398 factor:1 | -1 (0.44210) | -1 | -1 |
| G: -5254.59478 HOMO: -6.80285 LUMO: -0.55783 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11518.65704 HOMO: -6.82462 LUMO: 1.86670 factor:1 | -1 (0.30343) | -1 | -1 |
| G: -5254.59478 HOMO: -6.80285 LUMO: -0.55783 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11518.53709 HOMO: -6.83278 LUMO: 1.71160 factor:1 | -1 (0.42338) | -1 | -1 |
| G: -5254.59478 HOMO: -6.80285 LUMO: -0.55783 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11518.89767 HOMO: -6.62869 LUMO: 1.69527 factor:1 | -1 (0.06280) | -1 | -1 |
| G: -5254.59478 HOMO: -6.80285 LUMO: -0.55783 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11518.43940 HOMO: -6.84094 LUMO: 1.27349 factor:1 | -1 (0.52107) | -1 | -1 |
| G: -5254.59478 HOMO: -6.80285 LUMO: -0.55783 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11518.70839 HOMO: -7.07768 LUMO: 1.27621 factor:1 | -1 (0.25209) | 1 | -1 |
| G: -5254.59478 HOMO: -6.80285 LUMO: -0.55783 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11518.34005 HOMO: -7.06135 LUMO: 1.55105 factor:1 | -1 (0.62042) | 1 | -1 |
| G: -5254.59478 HOMO: -6.80285 LUMO: -0.55783 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11518.55614 HOMO: -6.94162 LUMO: 1.64629 factor:1 | -1 (0.40433) | -1 | -1 |
| G: -5254.59478 HOMO: -6.80285 LUMO: -0.55783 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11518.74558 HOMO: -7.07224 LUMO: 1.65445 factor:1 | -1 (0.21489) | 1 | -1 |
| G: -5254.59478 HOMO: -6.80285 LUMO: -0.55783 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11518.53361 HOMO: -6.68584 LUMO: 1.91296 factor:1 | -1 (0.42687) | -1 | -1 |
| G: -5254.59478 HOMO: -6.80285 LUMO: -0.55783 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11518.49701 HOMO: -7.09129 LUMO: 1.73609 factor:1 | -1 (0.46346) | 1 | -1 |
| G: -5254.59478 HOMO: -6.80285 LUMO: -0.55783 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11518.59464 HOMO: -7.01237 LUMO: 2.01092 factor:1 | -1 (0.36583) | -1 | -1 |
| G: -5254.59478 HOMO: -6.80285 LUMO: -0.55783 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11518.39883 HOMO: -6.93618 LUMO: 1.63540 factor:1 | -1 (0.56164) | -1 | -1 |
| G: -5254.59478 HOMO: -6.80285 LUMO: -0.55783 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11518.58882 HOMO: -6.98516 LUMO: 1.64629 factor:1 | -1 (0.37165) | -1 | -1 |
| G: -5254.59478 HOMO: -6.80285 LUMO: -0.55783 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11518.52174 HOMO: -6.80285 LUMO: 1.95106 factor:1 | -1 (0.43873) | -1 | -1 |
| G: -5254.59478 HOMO: -6.80285 LUMO: -0.55783 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11518.31407 HOMO: -6.76747 LUMO: 1.88303 factor:1 | -1 (0.64641) | -1 | -1 |
| G: -5254.59478 HOMO: -6.80285 LUMO: -0.55783 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11518.24770 HOMO: -6.64230 LUMO: 1.90480 factor:1 | -1 (0.71278) | -1 | -1 |
| G: -5254.59478 HOMO: -6.80285 LUMO: -0.55783 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11518.10878 HOMO: -6.93618 LUMO: 2.19324 factor:1 | -1 (0.85169) | -1 | -1 |
| G: -5254.59478 HOMO: -6.80285 LUMO: -0.55783 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11518.37622 HOMO: -6.95523 LUMO: 1.80684 factor:1 | -1 (0.58426) | -1 | -1 |
| G: -5254.59478 HOMO: -6.80285 LUMO: -0.55783 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11518.54457 HOMO: -6.66135 LUMO: 1.72792 factor:1 | -1 (0.41590) | -1 | -1 |
| G: -5254.59478 HOMO: -6.80285 LUMO: -0.55783 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11518.36506 HOMO: -6.36202 LUMO: 1.89391 factor:1 | -1 (0.59541) | -1 | -1 |
| G: -5254.59478 HOMO: -6.80285 LUMO: -0.55783 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11518.12702 HOMO: -7.03959 LUMO: 2.06262 factor:1 | -1 (0.83346) | -1 | -1 |
| G: -5254.59478 HOMO: -6.80285 LUMO: -0.55783 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11518.34465 HOMO: -7.08584 LUMO: 2.01092 factor:1 | -1 (0.61582) | 1 | -1 |
| G: -5253.59288 HOMO: -7.16476 LUMO: 2.86264 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11518.89160 HOMO: -6.96067 LUMO: 1.59731 factor:1 | 1 (-0.93302) | -1 | -1 |
| G: -5253.59288 HOMO: -7.16476 LUMO: 2.86264 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11518.65927 HOMO: -6.91169 LUMO: 1.37145 factor:1 | 1 (-0.70069) | -1 | -1 |
| G: -5253.59288 HOMO: -7.16476 LUMO: 2.86264 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11518.49086 HOMO: -6.94707 LUMO: 1.73064 factor:1 | 1 (-0.53228) | -1 | -1 |
| G: -5253.59288 HOMO: -7.16476 LUMO: 2.86264 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11518.83960 HOMO: -7.02326 LUMO: 1.41227 factor:1 | 1 (-0.88102) | -1 | -1 |
| G: -5253.59288 HOMO: -7.16476 LUMO: 2.86264 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11518.87878 HOMO: -6.72121 LUMO: 1.43132 factor:1 | 1 (-0.92021) | -1 | -1 |
| G: -5253.59288 HOMO: -7.16476 LUMO: 2.86264 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11518.53475 HOMO: -6.51168 LUMO: 1.72520 factor:1 | 1 (-0.57617) | -1 | -1 |
| G: -5253.59288 HOMO: -7.16476 LUMO: 2.86264 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11518.29701 HOMO: -6.98516 LUMO: 1.92929 factor:1 | 1 (-0.33843) | -1 | -1 |
| G: -5253.59288 HOMO: -7.16476 LUMO: 2.86264 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11518.16348 HOMO: -6.92802 LUMO: 2.07895 factor:1 | 1 (-0.20490) | -1 | -1 |
| G: -5253.59288 HOMO: -7.16476 LUMO: 2.86264 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11518.51837 HOMO: -7.02326 LUMO: 1.86398 factor:1 | 1 (-0.55979) | -1 | -1 |
| G: -5253.59288 HOMO: -7.16476 LUMO: 2.86264 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11518.65704 HOMO: -6.82462 LUMO: 1.86670 factor:1 | 1 (-0.69846) | -1 | -1 |
| G: -5253.59288 HOMO: -7.16476 LUMO: 2.86264 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11518.53709 HOMO: -6.83278 LUMO: 1.71160 factor:1 | 1 (-0.57851) | -1 | -1 |
| G: -5253.59288 HOMO: -7.16476 LUMO: 2.86264 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11518.89767 HOMO: -6.62869 LUMO: 1.69527 factor:1 | 1 (-0.93909) | -1 | -1 |
| G: -5253.59288 HOMO: -7.16476 LUMO: 2.86264 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11518.43940 HOMO: -6.84094 LUMO: 1.27349 factor:1 | 1 (-0.48083) | -1 | -1 |
| G: -5253.59288 HOMO: -7.16476 LUMO: 2.86264 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11518.70839 HOMO: -7.07768 LUMO: 1.27621 factor:1 | 1 (-0.74981) | -1 | -1 |
| G: -5253.59288 HOMO: -7.16476 LUMO: 2.86264 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11518.34005 HOMO: -7.06135 LUMO: 1.55105 factor:1 | 1 (-0.38148) | -1 | -1 |
| G: -5253.59288 HOMO: -7.16476 LUMO: 2.86264 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11518.55614 HOMO: -6.94162 LUMO: 1.64629 factor:1 | 1 (-0.59756) | -1 | -1 |
| G: -5253.59288 HOMO: -7.16476 LUMO: 2.86264 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11518.74558 HOMO: -7.07224 LUMO: 1.65445 factor:1 | 1 (-0.78701) | -1 | -1 |
| G: -5253.59288 HOMO: -7.16476 LUMO: 2.86264 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11518.53361 HOMO: -6.68584 LUMO: 1.91296 factor:1 | 1 (-0.57503) | -1 | -1 |
| G: -5253.59288 HOMO: -7.16476 LUMO: 2.86264 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11518.49701 HOMO: -7.09129 LUMO: 1.73609 factor:1 | 1 (-0.53843) | -1 | -1 |
| G: -5253.59288 HOMO: -7.16476 LUMO: 2.86264 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11518.59464 HOMO: -7.01237 LUMO: 2.01092 factor:1 | 1 (-0.63607) | -1 | -1 |
| G: -5253.59288 HOMO: -7.16476 LUMO: 2.86264 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11518.39883 HOMO: -6.93618 LUMO: 1.63540 factor:1 | 1 (-0.44025) | -1 | -1 |
| G: -5253.59288 HOMO: -7.16476 LUMO: 2.86264 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11518.58882 HOMO: -6.98516 LUMO: 1.64629 factor:1 | 1 (-0.63024) | -1 | -1 |
| G: -5253.59288 HOMO: -7.16476 LUMO: 2.86264 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11518.52174 HOMO: -6.80285 LUMO: 1.95106 factor:1 | 1 (-0.56317) | -1 | -1 |
| G: -5253.59288 HOMO: -7.16476 LUMO: 2.86264 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11518.31407 HOMO: -6.76747 LUMO: 1.88303 factor:1 | 1 (-0.35549) | -1 | -1 |
| G: -5253.59288 HOMO: -7.16476 LUMO: 2.86264 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11518.24770 HOMO: -6.64230 LUMO: 1.90480 factor:1 | 1 (-0.28912) | -1 | -1 |
| G: -5253.59288 HOMO: -7.16476 LUMO: 2.86264 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11518.10878 HOMO: -6.93618 LUMO: 2.19324 factor:1 | 1 (-0.15021) | -1 | -1 |
| G: -5253.59288 HOMO: -7.16476 LUMO: 2.86264 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11518.37622 HOMO: -6.95523 LUMO: 1.80684 factor:1 | 1 (-0.41764) | -1 | -1 |
| G: -5253.59288 HOMO: -7.16476 LUMO: 2.86264 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11518.54457 HOMO: -6.66135 LUMO: 1.72792 factor:1 | 1 (-0.58600) | -1 | -1 |
| G: -5253.59288 HOMO: -7.16476 LUMO: 2.86264 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11518.36506 HOMO: -6.36202 LUMO: 1.89391 factor:1 | 1 (-0.40648) | -1 | -1 |
| G: -5253.59288 HOMO: -7.16476 LUMO: 2.86264 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11518.12702 HOMO: -7.03959 LUMO: 2.06262 factor:1 | 1 (-0.16844) | -1 | -1 |
| G: -5253.59288 HOMO: -7.16476 LUMO: 2.86264 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11518.34465 HOMO: -7.08584 LUMO: 2.01092 factor:1 | 1 (-0.38608) | -1 | -1 |
| G: -5253.47615 HOMO: -6.50352 LUMO: 2.10888 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11518.89160 HOMO: -6.96067 LUMO: 1.59731 factor:1 | 1 (-1.04976) | 1 | 1 |
| G: -5253.47615 HOMO: -6.50352 LUMO: 2.10888 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11518.65927 HOMO: -6.91169 LUMO: 1.37145 factor:1 | 1 (-0.81743) | -1 | -1 |
| G: -5253.47615 HOMO: -6.50352 LUMO: 2.10888 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11518.49086 HOMO: -6.94707 LUMO: 1.73064 factor:1 | 1 (-0.64902) | 1 | 1 |
| G: -5253.47615 HOMO: -6.50352 LUMO: 2.10888 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11518.83960 HOMO: -7.02326 LUMO: 1.41227 factor:1 | 1 (-0.99776) | -1 | -1 |
| G: -5253.47615 HOMO: -6.50352 LUMO: 2.10888 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11518.87878 HOMO: -6.72121 LUMO: 1.43132 factor:1 | 1 (-1.03694) | -1 | -1 |
| G: -5253.47615 HOMO: -6.50352 LUMO: 2.10888 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11518.53475 HOMO: -6.51168 LUMO: 1.72520 factor:1 | 1 (-0.69291) | 1 | 1 |
| G: -5253.47615 HOMO: -6.50352 LUMO: 2.10888 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11518.29701 HOMO: -6.98516 LUMO: 1.92929 factor:1 | 1 (-0.45516) | 1 | 1 |
| G: -5253.47615 HOMO: -6.50352 LUMO: 2.10888 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11518.16348 HOMO: -6.92802 LUMO: 2.07895 factor:1 | 1 (-0.32164) | 1 | 1 |
| G: -5253.47615 HOMO: -6.50352 LUMO: 2.10888 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11518.51837 HOMO: -7.02326 LUMO: 1.86398 factor:1 | 1 (-0.67653) | 1 | 1 |
| G: -5253.47615 HOMO: -6.50352 LUMO: 2.10888 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11518.65704 HOMO: -6.82462 LUMO: 1.86670 factor:1 | 1 (-0.81520) | 1 | 1 |
| G: -5253.47615 HOMO: -6.50352 LUMO: 2.10888 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11518.53709 HOMO: -6.83278 LUMO: 1.71160 factor:1 | 1 (-0.69525) | 1 | 1 |
| G: -5253.47615 HOMO: -6.50352 LUMO: 2.10888 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11518.89767 HOMO: -6.62869 LUMO: 1.69527 factor:1 | 1 (-1.05583) | 1 | 1 |
| G: -5253.47615 HOMO: -6.50352 LUMO: 2.10888 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11518.43940 HOMO: -6.84094 LUMO: 1.27349 factor:1 | 1 (-0.59756) | -1 | -1 |
| G: -5253.47615 HOMO: -6.50352 LUMO: 2.10888 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11518.70839 HOMO: -7.07768 LUMO: 1.27621 factor:1 | 1 (-0.86655) | -1 | -1 |
| G: -5253.47615 HOMO: -6.50352 LUMO: 2.10888 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11518.34005 HOMO: -7.06135 LUMO: 1.55105 factor:1 | 1 (-0.49821) | -1 | -1 |
| G: -5253.47615 HOMO: -6.50352 LUMO: 2.10888 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11518.55614 HOMO: -6.94162 LUMO: 1.64629 factor:1 | 1 (-0.71430) | 1 | 1 |
| G: -5253.47615 HOMO: -6.50352 LUMO: 2.10888 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11518.74558 HOMO: -7.07224 LUMO: 1.65445 factor:1 | 1 (-0.90374) | 1 | 1 |
| G: -5253.47615 HOMO: -6.50352 LUMO: 2.10888 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11518.53361 HOMO: -6.68584 LUMO: 1.91296 factor:1 | 1 (-0.69177) | 1 | 1 |
| G: -5253.47615 HOMO: -6.50352 LUMO: 2.10888 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11518.49701 HOMO: -7.09129 LUMO: 1.73609 factor:1 | 1 (-0.65517) | 1 | 1 |
| G: -5253.47615 HOMO: -6.50352 LUMO: 2.10888 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11518.59464 HOMO: -7.01237 LUMO: 2.01092 factor:1 | 1 (-0.75280) | 1 | 1 |
| G: -5253.47615 HOMO: -6.50352 LUMO: 2.10888 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11518.39883 HOMO: -6.93618 LUMO: 1.63540 factor:1 | 1 (-0.55699) | 1 | 1 |
| G: -5253.47615 HOMO: -6.50352 LUMO: 2.10888 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11518.58882 HOMO: -6.98516 LUMO: 1.64629 factor:1 | 1 (-0.74698) | 1 | 1 |
| G: -5253.47615 HOMO: -6.50352 LUMO: 2.10888 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11518.52174 HOMO: -6.80285 LUMO: 1.95106 factor:1 | 1 (-0.67990) | 1 | 1 |
| G: -5253.47615 HOMO: -6.50352 LUMO: 2.10888 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11518.31407 HOMO: -6.76747 LUMO: 1.88303 factor:1 | 1 (-0.47223) | 1 | 1 |
| G: -5253.47615 HOMO: -6.50352 LUMO: 2.10888 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11518.24770 HOMO: -6.64230 LUMO: 1.90480 factor:1 | 1 (-0.40586) | 1 | 1 |
| G: -5253.47615 HOMO: -6.50352 LUMO: 2.10888 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11518.10878 HOMO: -6.93618 LUMO: 2.19324 factor:1 | 1 (-0.26694) | 1 | 1 |
| G: -5253.47615 HOMO: -6.50352 LUMO: 2.10888 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11518.37622 HOMO: -6.95523 LUMO: 1.80684 factor:1 | 1 (-0.53438) | 1 | 1 |
| G: -5253.47615 HOMO: -6.50352 LUMO: 2.10888 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11518.54457 HOMO: -6.66135 LUMO: 1.72792 factor:1 | 1 (-0.70273) | 1 | 1 |
| G: -5253.47615 HOMO: -6.50352 LUMO: 2.10888 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11518.36506 HOMO: -6.36202 LUMO: 1.89391 factor:1 | 1 (-0.52322) | -1 | -1 |
| G: -5253.47615 HOMO: -6.50352 LUMO: 2.10888 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11518.12702 HOMO: -7.03959 LUMO: 2.06262 factor:1 | 1 (-0.28518) | 1 | 1 |
| G: -5253.47615 HOMO: -6.50352 LUMO: 2.10888 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11518.34465 HOMO: -7.08584 LUMO: 2.01092 factor:1 | 1 (-0.50281) | 1 | 1 |
| G: -5253.45133 HOMO: -6.59604 LUMO: 2.33746 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11518.89160 HOMO: -6.96067 LUMO: 1.59731 factor:1 | 1 (-1.07458) | 1 | 1 |
| G: -5253.45133 HOMO: -6.59604 LUMO: 2.33746 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11518.65927 HOMO: -6.91169 LUMO: 1.37145 factor:1 | 1 (-0.84225) | -1 | -1 |
| G: -5253.45133 HOMO: -6.59604 LUMO: 2.33746 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11518.49086 HOMO: -6.94707 LUMO: 1.73064 factor:1 | 1 (-0.67384) | 1 | 1 |
| G: -5253.45133 HOMO: -6.59604 LUMO: 2.33746 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11518.83960 HOMO: -7.02326 LUMO: 1.41227 factor:1 | 1 (-1.02258) | -1 | -1 |
| G: -5253.45133 HOMO: -6.59604 LUMO: 2.33746 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11518.87878 HOMO: -6.72121 LUMO: 1.43132 factor:1 | 1 (-1.06176) | -1 | -1 |
| G: -5253.45133 HOMO: -6.59604 LUMO: 2.33746 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11518.53475 HOMO: -6.51168 LUMO: 1.72520 factor:1 | 1 (-0.71773) | -1 | -1 |
| G: -5253.45133 HOMO: -6.59604 LUMO: 2.33746 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11518.29701 HOMO: -6.98516 LUMO: 1.92929 factor:1 | 1 (-0.47998) | 1 | 1 |
| G: -5253.45133 HOMO: -6.59604 LUMO: 2.33746 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11518.16348 HOMO: -6.92802 LUMO: 2.07895 factor:1 | 1 (-0.34646) | 1 | 1 |
| G: -5253.45133 HOMO: -6.59604 LUMO: 2.33746 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11518.51837 HOMO: -7.02326 LUMO: 1.86398 factor:1 | 1 (-0.70135) | 1 | 1 |
| G: -5253.45133 HOMO: -6.59604 LUMO: 2.33746 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11518.65704 HOMO: -6.82462 LUMO: 1.86670 factor:1 | 1 (-0.84002) | 1 | 1 |
| G: -5253.45133 HOMO: -6.59604 LUMO: 2.33746 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11518.53709 HOMO: -6.83278 LUMO: 1.71160 factor:1 | 1 (-0.72007) | 1 | 1 |
| G: -5253.45133 HOMO: -6.59604 LUMO: 2.33746 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11518.89767 HOMO: -6.62869 LUMO: 1.69527 factor:1 | 1 (-1.08065) | 1 | 1 |
| G: -5253.45133 HOMO: -6.59604 LUMO: 2.33746 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11518.43940 HOMO: -6.84094 LUMO: 1.27349 factor:1 | 1 (-0.62238) | -1 | -1 |
| G: -5253.45133 HOMO: -6.59604 LUMO: 2.33746 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11518.70839 HOMO: -7.07768 LUMO: 1.27621 factor:1 | 1 (-0.89136) | -1 | -1 |
| G: -5253.45133 HOMO: -6.59604 LUMO: 2.33746 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11518.34005 HOMO: -7.06135 LUMO: 1.55105 factor:1 | 1 (-0.52303) | -1 | -1 |
| G: -5253.45133 HOMO: -6.59604 LUMO: 2.33746 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11518.55614 HOMO: -6.94162 LUMO: 1.64629 factor:1 | 1 (-0.73912) | 1 | 1 |
| G: -5253.45133 HOMO: -6.59604 LUMO: 2.33746 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11518.74558 HOMO: -7.07224 LUMO: 1.65445 factor:1 | 1 (-0.92856) | 1 | 1 |
| G: -5253.45133 HOMO: -6.59604 LUMO: 2.33746 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11518.53361 HOMO: -6.68584 LUMO: 1.91296 factor:1 | 1 (-0.71658) | 1 | 1 |
| G: -5253.45133 HOMO: -6.59604 LUMO: 2.33746 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11518.49701 HOMO: -7.09129 LUMO: 1.73609 factor:1 | 1 (-0.67999) | 1 | 1 |
| G: -5253.45133 HOMO: -6.59604 LUMO: 2.33746 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11518.59464 HOMO: -7.01237 LUMO: 2.01092 factor:1 | 1 (-0.77762) | 1 | 1 |
| G: -5253.45133 HOMO: -6.59604 LUMO: 2.33746 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11518.39883 HOMO: -6.93618 LUMO: 1.63540 factor:1 | 1 (-0.58181) | 1 | 1 |
| G: -5253.45133 HOMO: -6.59604 LUMO: 2.33746 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11518.58882 HOMO: -6.98516 LUMO: 1.64629 factor:1 | 1 (-0.77180) | 1 | 1 |
| G: -5253.45133 HOMO: -6.59604 LUMO: 2.33746 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11518.52174 HOMO: -6.80285 LUMO: 1.95106 factor:1 | 1 (-0.70472) | 1 | 1 |
| G: -5253.45133 HOMO: -6.59604 LUMO: 2.33746 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11518.31407 HOMO: -6.76747 LUMO: 1.88303 factor:1 | 1 (-0.49704) | 1 | 1 |
| G: -5253.45133 HOMO: -6.59604 LUMO: 2.33746 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11518.24770 HOMO: -6.64230 LUMO: 1.90480 factor:1 | 1 (-0.43067) | 1 | 1 |
| G: -5253.45133 HOMO: -6.59604 LUMO: 2.33746 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11518.10878 HOMO: -6.93618 LUMO: 2.19324 factor:1 | 1 (-0.29176) | 1 | 1 |
| G: -5253.45133 HOMO: -6.59604 LUMO: 2.33746 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11518.37622 HOMO: -6.95523 LUMO: 1.80684 factor:1 | 1 (-0.55919) | 1 | 1 |
| G: -5253.45133 HOMO: -6.59604 LUMO: 2.33746 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11518.54457 HOMO: -6.66135 LUMO: 1.72792 factor:1 | 1 (-0.72755) | 1 | 1 |
| G: -5253.45133 HOMO: -6.59604 LUMO: 2.33746 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11518.36506 HOMO: -6.36202 LUMO: 1.89391 factor:1 | 1 (-0.54804) | -1 | -1 |
| G: -5253.45133 HOMO: -6.59604 LUMO: 2.33746 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11518.12702 HOMO: -7.03959 LUMO: 2.06262 factor:1 | 1 (-0.30999) | 1 | 1 |
| G: -5253.45133 HOMO: -6.59604 LUMO: 2.33746 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11518.34465 HOMO: -7.08584 LUMO: 2.01092 factor:1 | 1 (-0.52763) | 1 | 1 |
| G: -4176.47485 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -5220.16791 HOMO: -7.06135 LUMO: 0.75376 factor:2 | -1 (0.50472) | 1 | -1 |
| G: -4176.47485 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10444.10613 HOMO: -5.10213 LUMO: 0.77825 factor:1 | 1 (-3.26558) | -1 | -1 |
| G: -4176.47485 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10443.76000 HOMO: -5.84228 LUMO: 0.50341 factor:1 | 1 (-2.91946) | -1 | -1 |
| G: -4176.47485 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10443.80928 HOMO: -5.39874 LUMO: 0.68028 factor:1 | 1 (-2.96874) | -1 | -1 |
| G: -4176.47485 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10443.63855 HOMO: -5.16744 LUMO: 1.14832 factor:1 | 1 (-2.79801) | -1 | -1 |
| G: -4176.47485 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10443.88819 HOMO: -5.80963 LUMO: 0.35647 factor:1 | 1 (-3.04765) | -1 | -1 |
| G: -4176.47485 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10443.75679 HOMO: -5.02322 LUMO: 1.07213 factor:1 | 1 (-2.91624) | -1 | -1 |
| G: -4176.47485 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10443.79325 HOMO: -5.80963 LUMO: 0.56328 factor:1 | 1 (-2.95271) | -1 | -1 |
| G: -4176.47485 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10443.58002 HOMO: -5.45316 LUMO: 0.78369 factor:1 | 1 (-2.73948) | -1 | -1 |
| G: -4176.47485 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10444.00085 HOMO: -5.25452 LUMO: 0.82178 factor:1 | 1 (-3.16030) | -1 | -1 |
| G: -4176.47485 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10443.63904 HOMO: -5.21370 LUMO: 1.03947 factor:1 | 1 (-2.79850) | -1 | -1 |
| G: -4176.47485 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10443.35264 HOMO: -6.04365 LUMO: 0.31837 factor:1 | 1 (-2.51210) | -1 | -1 |
| G: -4176.47485 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10443.66032 HOMO: -5.86405 LUMO: 0.55511 factor:1 | 1 (-2.81978) | -1 | -1 |
| G: -4176.47485 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10443.45333 HOMO: -5.64908 LUMO: 0.71022 factor:1 | 1 (-2.61278) | -1 | -1 |
| G: -4176.47485 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10443.29678 HOMO: -5.94297 LUMO: 0.68301 factor:1 | 1 (-2.45624) | -1 | -1 |
| G: -4176.47485 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10443.54900 HOMO: -6.01916 LUMO: 0.56328 factor:1 | 1 (-2.70846) | -1 | -1 |
| G: -4176.47485 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10443.75230 HOMO: -6.05181 LUMO: 0.35103 factor:1 | 1 (-2.91175) | -1 | -1 |
| G: -4176.47485 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10443.64971 HOMO: -6.08447 LUMO: 0.48436 factor:1 | 1 (-2.80917) | -1 | -1 |
| G: -4176.47485 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10443.74851 HOMO: -5.86950 LUMO: 0.36735 factor:1 | 1 (-2.90797) | -1 | -1 |
| G: -4176.47485 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10443.81189 HOMO: -5.33615 LUMO: 0.65852 factor:1 | 1 (-2.97135) | -1 | -1 |
| G: -4176.47485 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10443.61161 HOMO: -5.36064 LUMO: 0.86804 factor:1 | 1 (-2.77107) | -1 | -1 |
| G: -4176.47485 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10443.73831 HOMO: -5.74160 LUMO: 0.64491 factor:1 | 1 (-2.89777) | -1 | -1 |
| G: -4176.47485 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10443.53093 HOMO: -5.23003 LUMO: 0.66124 factor:1 | 1 (-2.69039) | -1 | -1 |
| G: -4176.47485 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10443.64280 HOMO: -5.77698 LUMO: 0.84083 factor:1 | 1 (-2.80226) | -1 | -1 |
| G: -4176.47485 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10443.47520 HOMO: -5.60555 LUMO: 0.84355 factor:1 | 1 (-2.63466) | -1 | -1 |
| G: -4176.47485 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10442.52920 HOMO: -7.11578 LUMO: -1.62452 factor:1 | 1 (-1.68866) | -1 | -1 |
| G: -4176.47485 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10442.45284 HOMO: -7.23279 LUMO: -1.63813 factor:1 | 1 (-1.61230) | -1 | -1 |
| G: -4176.47485 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10442.61736 HOMO: -6.68312 LUMO: -0.88709 factor:1 | 1 (-1.77682) | -1 | -1 |
| G: -4176.47485 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10442.40046 HOMO: -6.99333 LUMO: -0.88709 factor:1 | 1 (-1.55992) | -1 | -1 |
| G: -4176.47485 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10442.65481 HOMO: -7.40694 LUMO: 0.11973 factor:1 | 1 (-1.81426) | 1 | 1 |
| G: -4176.47485 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10442.23420 HOMO: -6.74026 LUMO: -0.72927 factor:1 | 1 (-1.39366) | -1 | -1 |
| G: -4176.47485 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10442.56008 HOMO: -6.67223 LUMO: -0.70750 factor:1 | 1 (-1.71954) | -1 | -1 |
| G: -4176.47485 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10442.77269 HOMO: -7.06952 LUMO: -1.40139 factor:1 | 1 (-1.93214) | -1 | -1 |
| G: -4176.47485 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10444.65803 HOMO: -7.21374 LUMO: -1.13199 factor:1 | 1 (-3.81749) | -1 | -1 |
| G: -4176.47485 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10443.96414 HOMO: -6.54706 LUMO: -1.34424 factor:1 | 1 (-3.12360) | -1 | -1 |
| G: -4176.47485 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10443.11691 HOMO: -7.51851 LUMO: -1.05852 factor:1 | 1 (-2.27637) | -1 | -1 |
| G: -4176.47485 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10442.57230 HOMO: -7.07224 LUMO: -1.89391 factor:1 | 1 (-1.73176) | -1 | -1 |
| G: -4176.47485 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10442.49540 HOMO: -6.65863 LUMO: -0.46804 factor:1 | 1 (-1.65486) | -1 | -1 |
| G: -4176.47485 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10443.24048 HOMO: -7.24367 LUMO: 0.29388 factor:1 | 1 (-2.39994) | 1 | 1 |
| G: -4176.47485 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10443.60008 HOMO: -7.02326 LUMO: -0.87893 factor:1 | 1 (-2.75953) | -1 | -1 |
| G: -4176.47485 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10441.50382 HOMO: -6.88176 LUMO: 0.71566 factor:1 | 1 (-0.66328) | -1 | -1 |
| G: -4176.47485 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10441.43163 HOMO: -6.46543 LUMO: 1.01498 factor:1 | 1 (-0.59109) | -1 | -1 |
| G: -4176.47485 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10441.80257 HOMO: -6.30760 LUMO: 0.17687 factor:1 | 1 (-0.96203) | -1 | -1 |
| G: -4176.47485 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10441.52281 HOMO: -6.73210 LUMO: -1.06941 factor:1 | 1 (-0.68227) | -1 | -1 |
| G: -4176.47485 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10441.85174 HOMO: -6.83550 LUMO: -0.75920 factor:1 | 1 (-1.01120) | -1 | -1 |
| G: -4176.47485 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10443.50644 HOMO: -6.94707 LUMO: 0.42178 factor:1 | 1 (-2.66590) | -1 | -1 |
| G: -4176.47485 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10442.06976 HOMO: -6.77019 LUMO: -0.38096 factor:1 | 1 (-1.22922) | -1 | -1 |
| G: -4176.47485 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10443.26989 HOMO: -7.34163 LUMO: 0.35103 factor:1 | 1 (-2.42935) | 1 | 1 |
| G: -4176.47485 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10442.48849 HOMO: -6.87632 LUMO: -0.87349 factor:1 | 1 (-1.64795) | -1 | -1 |
| G: -4176.47485 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10442.50313 HOMO: -7.06952 LUMO: -1.47214 factor:1 | 1 (-1.66259) | -1 | -1 |
| G: -4176.47485 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10442.60036 HOMO: -6.58788 LUMO: -0.37824 factor:1 | 1 (-1.75981) | -1 | -1 |
| G: -4176.47485 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10442.73832 HOMO: -6.92802 LUMO: -1.24900 factor:1 | 1 (-1.89778) | -1 | -1 |
| G: -4176.47485 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10442.33815 HOMO: -7.01237 LUMO: -1.31975 factor:1 | 1 (-1.49761) | -1 | -1 |
| G: -4176.47485 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10441.41334 HOMO: -6.74842 LUMO: 0.45987 factor:1 | 1 (-0.57280) | -1 | -1 |
| G: -4176.47485 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10441.53130 HOMO: -6.53890 LUMO: 0.94424 factor:1 | 1 (-0.69076) | -1 | -1 |
| G: -4176.47485 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10443.68394 HOMO: -6.52257 LUMO: -0.66940 factor:1 | 1 (-2.84340) | -1 | -1 |
| G: -4176.47485 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10444.02264 HOMO: -6.56883 LUMO: -1.48302 factor:1 | 1 (-3.18210) | -1 | -1 |
| G: -4176.47485 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10443.13302 HOMO: -7.21646 LUMO: 0.13061 factor:1 | 1 (-2.29248) | 1 | 1 |
| G: -4176.47485 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10442.51627 HOMO: -6.62597 LUMO: -0.64763 factor:1 | 1 (-1.67573) | -1 | -1 |
| G: -4176.47485 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10442.87707 HOMO: -7.38789 LUMO: 0.31021 factor:1 | 1 (-2.03653) | 1 | 1 |
| G: -4176.47485 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10442.20587 HOMO: -6.74570 LUMO: -0.70750 factor:1 | 1 (-1.36533) | -1 | -1 |
| G: -4176.47485 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10442.81688 HOMO: -6.95251 LUMO: -1.25989 factor:1 | 1 (-1.97634) | -1 | -1 |
| G: -4176.47485 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10443.51504 HOMO: -7.13483 LUMO: -0.76736 factor:1 | 1 (-2.67450) | -1 | -1 |
| G: -4176.47485 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10442.41959 HOMO: -6.93618 LUMO: -1.24628 factor:1 | 1 (-1.57905) | -1 | -1 |
| G: -4176.47485 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10443.14586 HOMO: -7.03686 LUMO: 0.26395 factor:1 | 1 (-2.30532) | -1 | -1 |
| G: -4176.47485 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10442.05025 HOMO: -6.52257 LUMO: -0.84355 factor:1 | 1 (-1.20971) | -1 | -1 |
| G: -4176.47485 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10442.44283 HOMO: -6.83278 LUMO: -0.49525 factor:1 | 1 (-1.60229) | -1 | -1 |
| G: -4176.47485 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10443.01473 HOMO: -7.18381 LUMO: -1.64629 factor:1 | 1 (-2.17419) | -1 | -1 |
| G: -4176.47485 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10442.94279 HOMO: -6.74842 LUMO: -0.81090 factor:1 | 1 (-2.10224) | -1 | -1 |
| G: -4176.47485 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10442.59078 HOMO: -7.09401 LUMO: -0.92519 factor:1 | 1 (-1.75024) | -1 | -1 |
| G: -4176.47485 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10442.67965 HOMO: -7.20285 LUMO: -0.81634 factor:1 | 1 (-1.83911) | -1 | -1 |
| G: -4176.47485 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10441.60847 HOMO: -6.72665 LUMO: 0.77008 factor:1 | 1 (-0.76793) | -1 | -1 |
| G: -4176.47485 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10441.35574 HOMO: -6.80829 LUMO: 0.86532 factor:1 | 1 (-0.51519) | -1 | -1 |
| G: -4176.47485 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10441.70627 HOMO: -6.20964 LUMO: 0.99866 factor:1 | 1 (-0.86573) | -1 | -1 |
| G: -4176.47485 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10441.39767 HOMO: -6.52801 LUMO: 1.07757 factor:1 | 1 (-0.55713) | -1 | -1 |
| G: -4176.47485 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10443.87951 HOMO: -6.74298 LUMO: -0.67756 factor:1 | 1 (-3.03897) | -1 | -1 |
| G: -4176.47485 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10443.07950 HOMO: -7.43959 LUMO: 0.03265 factor:1 | 1 (-2.23895) | 1 | 1 |
| G: -4176.47485 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10442.62572 HOMO: -6.46815 LUMO: -0.29933 factor:1 | 1 (-1.78518) | -1 | -1 |
| G: -4176.47485 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10444.54224 HOMO: -6.70489 LUMO: -0.97145 factor:1 | 1 (-3.70170) | -1 | -1 |
| G: -4176.47485 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10443.77175 HOMO: -6.30216 LUMO: -1.39322 factor:1 | 1 (-2.93121) | -1 | -1 |
| G: -4176.47485 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10444.50491 HOMO: -7.01782 LUMO: -1.07485 factor:1 | 1 (-3.66437) | -1 | -1 |
| G: -4176.47485 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10444.38899 HOMO: -6.93074 LUMO: 0.25851 factor:1 | 1 (-3.54845) | -1 | -1 |
| G: -4176.47485 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10444.33631 HOMO: -7.07224 LUMO: 0.09524 factor:1 | 1 (-3.49577) | 1 | 1 |
| G: -4176.47485 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10443.72653 HOMO: -6.62325 LUMO: -0.45443 factor:1 | 1 (-2.88599) | -1 | -1 |
| G: -4176.47485 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10444.43805 HOMO: -7.09945 LUMO: -1.20274 factor:1 | 1 (-3.59751) | -1 | -1 |
| G: -4176.47485 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10443.92882 HOMO: -6.56067 LUMO: -1.39322 factor:1 | 1 (-3.08827) | -1 | -1 |
| G: -4176.47485 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10443.85975 HOMO: -6.75387 LUMO: -0.72654 factor:1 | 1 (-3.01921) | -1 | -1 |
| G: -4176.47485 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10444.21043 HOMO: -6.28583 LUMO: -2.35651 factor:1 | 1 (-3.36989) | -1 | -1 |
| G: -4176.47485 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10444.10923 HOMO: -6.55522 LUMO: -1.33608 factor:1 | 1 (-3.26869) | -1 | -1 |
| G: -4176.47485 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10444.79999 HOMO: -7.19741 LUMO: -0.93607 factor:1 | 1 (-3.95945) | -1 | -1 |
| G: -4176.47485 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10444.08218 HOMO: -6.39740 LUMO: -1.14832 factor:1 | 1 (-3.24164) | -1 | -1 |
| G: -4176.47485 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10444.78130 HOMO: -7.11850 LUMO: -0.97417 factor:1 | 1 (-3.94075) | -1 | -1 |
| G: -4176.47485 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10444.55501 HOMO: -6.57699 LUMO: -1.14016 factor:1 | 1 (-3.71446) | -1 | -1 |
| G: -4176.47485 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10444.15481 HOMO: -6.57699 LUMO: -1.31975 factor:1 | 1 (-3.31427) | -1 | -1 |
| G: -4176.47485 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10442.66248 HOMO: -6.69128 LUMO: -0.76736 factor:1 | 1 (-1.82194) | -1 | -1 |
| G: -4176.47485 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10443.57545 HOMO: -7.25728 LUMO: 0.29660 factor:1 | 1 (-2.73491) | 1 | 1 |
| G: -4176.47485 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10442.41129 HOMO: -6.37019 LUMO: -0.95240 factor:1 | 1 (-1.57075) | -1 | -1 |
| G: -4176.47485 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10442.68580 HOMO: -6.48447 LUMO: -0.55511 factor:1 | 1 (-1.84526) | -1 | -1 |
| G: -4176.47485 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10441.45525 HOMO: -6.37291 LUMO: -0.78641 factor:1 | 1 (-0.61471) | -1 | -1 |
| G: -4176.47485 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10441.71969 HOMO: -6.65863 LUMO: -0.69933 factor:1 | 1 (-0.87915) | -1 | -1 |
| G: -4176.47485 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10442.73903 HOMO: -6.44638 LUMO: -0.16055 factor:1 | 1 (-1.89848) | -1 | -1 |
| G: -4176.47485 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10442.62735 HOMO: -6.41917 LUMO: -0.20136 factor:1 | 1 (-1.78681) | -1 | -1 |
| G: -4176.47485 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10443.27071 HOMO: -7.33347 LUMO: 0.12789 factor:1 | 1 (-2.43017) | 1 | 1 |
| G: -4176.47485 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10443.61635 HOMO: -6.70489 LUMO: -0.52518 factor:1 | 1 (-2.77581) | -1 | -1 |
| G: -4176.47485 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10444.06770 HOMO: -7.25183 LUMO: 0.32109 factor:1 | 1 (-3.22716) | 1 | 1 |
| G: -4176.47485 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10443.95886 HOMO: -7.29265 LUMO: 0.28028 factor:1 | 1 (-3.11832) | 1 | 1 |
| G: -4176.47485 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10443.40426 HOMO: -6.57155 LUMO: -0.51702 factor:1 | 1 (-2.56372) | -1 | -1 |
| G: -4176.47485 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10443.63017 HOMO: -7.08040 LUMO: 0.39729 factor:1 | 1 (-2.78963) | 1 | 1 |
| G: -4176.47485 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10443.01998 HOMO: -6.24501 LUMO: -0.44627 factor:1 | 1 (-2.17944) | -1 | -1 |
| G: -4176.47485 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10443.28970 HOMO: -6.73754 LUMO: -0.45443 factor:1 | 1 (-2.44916) | -1 | -1 |
| G: -4176.47485 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10442.53105 HOMO: -6.24501 LUMO: 0.38096 factor:1 | 1 (-1.69051) | -1 | -1 |
| G: -4176.47485 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10443.46029 HOMO: -6.86815 LUMO: -0.91974 factor:1 | 1 (-2.61975) | -1 | -1 |
| G: -4176.47485 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10443.59404 HOMO: -7.40150 LUMO: 0.36191 factor:1 | 1 (-2.75349) | 1 | 1 |
| G: -4176.47485 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10442.68221 HOMO: -6.44094 LUMO: -0.64219 factor:1 | 1 (-1.84167) | -1 | -1 |
| G: -4176.47485 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10442.52321 HOMO: -6.69944 LUMO: -0.80001 factor:1 | 1 (-1.68267) | -1 | -1 |
| G: -4176.47485 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10441.33429 HOMO: -6.61509 LUMO: -0.70750 factor:1 | 1 (-0.49375) | -1 | -1 |
| G: -4176.47485 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10442.25820 HOMO: -7.52123 LUMO: 0.06803 factor:1 | 1 (-1.41766) | 1 | 1 |
| G: -4176.47485 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10443.38894 HOMO: -7.34163 LUMO: 0.30477 factor:1 | 1 (-2.54840) | 1 | 1 |
| G: -4176.47485 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10442.75519 HOMO: -6.68584 LUMO: -0.78641 factor:1 | 1 (-1.91465) | -1 | -1 |
| G: -4176.47485 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10442.56180 HOMO: -6.53890 LUMO: -0.50885 factor:1 | 1 (-1.72126) | -1 | -1 |
| G: -4176.47485 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10441.59313 HOMO: -6.75659 LUMO: -0.68845 factor:1 | 1 (-0.75259) | -1 | -1 |
| G: -4176.47485 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10443.70345 HOMO: -7.08857 LUMO: 0.43266 factor:1 | 1 (-2.86291) | 1 | 1 |
| G: -4176.47485 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10442.98368 HOMO: -6.28583 LUMO: -0.46804 factor:1 | 1 (-2.14314) | -1 | -1 |
| G: -4176.47485 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10443.16499 HOMO: -6.50080 LUMO: -0.24762 factor:1 | 1 (-2.32445) | -1 | -1 |
| G: -4176.47485 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10442.81541 HOMO: -6.45454 LUMO: -0.58504 factor:1 | 1 (-1.97487) | -1 | -1 |
| G: -4176.47485 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10443.35398 HOMO: -7.20558 LUMO: 0.20953 factor:1 | 1 (-2.51343) | 1 | 1 |
| G: -4176.47485 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10442.75443 HOMO: -6.35930 LUMO: -0.20681 factor:1 | 1 (-1.91389) | -1 | -1 |
| G: -4176.47485 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10442.76945 HOMO: -6.36202 LUMO: -0.14422 factor:1 | 1 (-1.92891) | -1 | -1 |
| G: -4176.47485 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10440.43164 HOMO: -6.20692 LUMO: 1.97827 factor:1 | -1 (0.40891) | -1 | -1 |
| G: -4176.47485 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10440.24026 HOMO: -6.48719 LUMO: 1.74153 factor:1 | -1 (0.60028) | -1 | -1 |
| G: -4176.47485 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10440.74974 HOMO: -6.84638 LUMO: 1.88575 factor:1 | -1 (0.09080) | -1 | -1 |
| G: -4176.47485 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10441.06626 HOMO: -5.90759 LUMO: 2.00820 factor:1 | 1 (-0.22572) | -1 | -1 |
| G: -4176.47485 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10441.28066 HOMO: -6.56339 LUMO: 1.99732 factor:1 | 1 (-0.44012) | -1 | -1 |
| G: -4176.47485 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10440.22736 HOMO: -6.20692 LUMO: 1.75241 factor:1 | -1 (0.61318) | -1 | -1 |
| G: -4176.47485 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10440.40824 HOMO: -6.16882 LUMO: 1.94017 factor:1 | -1 (0.43231) | -1 | -1 |
| G: -4176.47485 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10440.68438 HOMO: -6.80829 LUMO: 1.78507 factor:1 | -1 (0.15617) | -1 | -1 |
| G: -4176.47485 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10441.46782 HOMO: -6.58243 LUMO: 1.78235 factor:1 | 1 (-0.62728) | -1 | -1 |
| G: -4176.47485 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10441.06713 HOMO: -5.85045 LUMO: 1.82316 factor:1 | 1 (-0.22659) | -1 | -1 |
| G: -4176.47485 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10441.20052 HOMO: -5.93752 LUMO: 1.56465 factor:1 | 1 (-0.35998) | -1 | -1 |
| G: -4176.47485 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10443.28565 HOMO: -6.59604 LUMO: -0.53334 factor:1 | 1 (-2.44511) | -1 | -1 |
| G: -4176.47485 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10443.78724 HOMO: -7.06135 LUMO: 0.29660 factor:1 | 1 (-2.94669) | 1 | 1 |
| G: -4176.47485 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10439.29861 HOMO: -6.50352 LUMO: 1.61908 factor:1 | -1 (1.54193) | -1 | -1 |
| G: -4176.47485 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10442.08021 HOMO: -6.68040 LUMO: -0.60681 factor:1 | 1 (-1.23967) | -1 | -1 |
| G: -4176.47485 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10442.19583 HOMO: -6.93618 LUMO: -1.09662 factor:1 | 1 (-1.35529) | -1 | -1 |
| G: -4176.47485 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10441.81041 HOMO: -6.72121 LUMO: -1.14016 factor:1 | 1 (-0.96987) | -1 | -1 |
| G: -4176.47485 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10442.28413 HOMO: -7.12394 LUMO: -1.24900 factor:1 | 1 (-1.44359) | -1 | -1 |
| G: -4176.47485 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10442.14808 HOMO: -6.71305 LUMO: -0.71566 factor:1 | 1 (-1.30753) | -1 | -1 |
| G: -4176.47485 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10442.52294 HOMO: -7.09401 LUMO: -0.86532 factor:1 | 1 (-1.68240) | -1 | -1 |
| G: -4176.47485 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10442.56324 HOMO: -7.08584 LUMO: -0.92519 factor:1 | 1 (-1.72270) | -1 | -1 |
| G: -4176.47485 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10443.05612 HOMO: -7.05591 LUMO: 0.11973 factor:1 | 1 (-2.21558) | -1 | -1 |
| G: -4176.47485 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10442.33069 HOMO: -7.14843 LUMO: -1.58370 factor:1 | 1 (-1.49015) | -1 | -1 |
| G: -4176.47485 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10442.53870 HOMO: -7.36884 LUMO: -1.97010 factor:1 | 1 (-1.69815) | -1 | -1 |
| G: -4176.47485 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10442.12375 HOMO: -6.81373 LUMO: -1.72248 factor:1 | 1 (-1.28321) | -1 | -1 |
| G: -4176.47485 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10442.71402 HOMO: -6.87360 LUMO: -1.03947 factor:1 | 1 (-1.87348) | -1 | -1 |
| G: -4176.47485 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10441.90919 HOMO: -7.02870 LUMO: -0.87349 factor:1 | 1 (-1.06865) | -1 | -1 |
| G: -4176.47485 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10442.35257 HOMO: -7.16476 LUMO: -1.18097 factor:1 | 1 (-1.51203) | -1 | -1 |
| G: -4176.47485 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10442.76156 HOMO: -7.51851 LUMO: 0.07891 factor:1 | 1 (-1.92102) | 1 | 1 |
| G: -4176.47485 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10441.88968 HOMO: -7.04231 LUMO: -0.83539 factor:1 | 1 (-1.04913) | -1 | -1 |
| G: -4176.47485 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10442.18315 HOMO: -6.83278 LUMO: -0.60137 factor:1 | 1 (-1.34261) | -1 | -1 |
| G: -4176.47485 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10442.59652 HOMO: -6.89809 LUMO: -1.19186 factor:1 | 1 (-1.75598) | -1 | -1 |
| G: -4176.47485 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10443.28728 HOMO: -7.16476 LUMO: -0.79185 factor:1 | 1 (-2.44674) | -1 | -1 |
| G: -4176.47485 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10442.56928 HOMO: -6.97156 LUMO: -1.25444 factor:1 | 1 (-1.72874) | -1 | -1 |
| G: -4176.47485 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10442.36547 HOMO: -6.84366 LUMO: -0.88437 factor:1 | 1 (-1.52493) | -1 | -1 |
| G: -4176.47485 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10442.53497 HOMO: -6.91986 LUMO: -1.12655 factor:1 | 1 (-1.69443) | -1 | -1 |
| G: -4176.47485 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10442.57837 HOMO: -6.49536 LUMO: -0.29660 factor:1 | 1 (-1.73783) | -1 | -1 |
| G: -4176.47485 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10443.39920 HOMO: -6.74842 LUMO: 0.42450 factor:1 | 1 (-2.55866) | -1 | -1 |
| G: -4176.47485 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10443.12834 HOMO: -7.34435 LUMO: 0.32109 factor:1 | 1 (-2.28780) | 1 | 1 |
| G: -4176.47485 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10443.17814 HOMO: -7.16476 LUMO: 0.28572 factor:1 | 1 (-2.33759) | 1 | 1 |
| G: -4176.47485 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10442.36375 HOMO: -6.74298 LUMO: -0.43538 factor:1 | 1 (-1.52321) | -1 | -1 |
| G: -4176.47485 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10442.40892 HOMO: -7.19469 LUMO: -1.61091 factor:1 | 1 (-1.56838) | -1 | -1 |
| G: -4176.47485 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10442.41246 HOMO: -7.35252 LUMO: -1.78235 factor:1 | 1 (-1.57192) | -1 | -1 |
| G: -4176.47485 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10442.07559 HOMO: -7.25456 LUMO: -1.66806 factor:1 | 1 (-1.23504) | -1 | -1 |
| G: -4176.47485 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10442.99628 HOMO: -7.54844 LUMO: -1.07213 factor:1 | 1 (-2.15574) | -1 | -1 |
| G: -4176.47485 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10442.10081 HOMO: -7.21918 LUMO: -1.55377 factor:1 | 1 (-1.26027) | -1 | -1 |
| G: -4176.47485 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10442.12130 HOMO: -7.01782 LUMO: -1.60547 factor:1 | 1 (-1.28076) | -1 | -1 |
| G: -4176.47485 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10442.32291 HOMO: -7.21646 LUMO: -1.53472 factor:1 | 1 (-1.48237) | -1 | -1 |
| G: -4176.47485 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10443.63284 HOMO: -6.73754 LUMO: -1.37417 factor:1 | 1 (-2.79230) | -1 | -1 |
| G: -4176.47485 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10441.42012 HOMO: -6.78924 LUMO: 0.66396 factor:1 | 1 (-0.57958) | -1 | -1 |
| G: -4176.47485 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10441.43285 HOMO: -6.82734 LUMO: 0.61226 factor:1 | 1 (-0.59231) | -1 | -1 |
| G: -4176.47485 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10441.61008 HOMO: -6.74026 LUMO: 0.65579 factor:1 | 1 (-0.76954) | -1 | -1 |
| G: -4176.47485 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10443.37161 HOMO: -7.10489 LUMO: -1.30887 factor:1 | 1 (-2.53107) | -1 | -1 |
| G: -4176.47485 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10441.44183 HOMO: -7.05047 LUMO: 0.42722 factor:1 | 1 (-0.60129) | -1 | -1 |
| G: -4176.47485 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10441.43440 HOMO: -6.61237 LUMO: 1.30887 factor:1 | 1 (-0.59386) | -1 | -1 |
| G: -4176.47485 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10441.36047 HOMO: -7.05863 LUMO: 0.59049 factor:1 | 1 (-0.51993) | -1 | -1 |
| G: -4176.47485 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10441.01774 HOMO: -6.26406 LUMO: 0.78641 factor:1 | 1 (-0.17720) | -1 | -1 |
| G: -4176.47485 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10441.35451 HOMO: -6.70489 LUMO: 0.67756 factor:1 | 1 (-0.51397) | -1 | -1 |
| G: -4176.47485 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10443.55512 HOMO: -6.78652 LUMO: -0.94968 factor:1 | 1 (-2.71458) | -1 | -1 |
| G: -4176.47485 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10443.35561 HOMO: -6.36202 LUMO: -0.94424 factor:1 | 1 (-2.51507) | -1 | -1 |
| G: -4176.47485 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10443.56623 HOMO: -6.81645 LUMO: -1.09934 factor:1 | 1 (-2.72568) | -1 | -1 |
| G: -4176.47485 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10441.97055 HOMO: -7.07224 LUMO: 0.85988 factor:1 | 1 (-1.13001) | 1 | 1 |
| G: -4176.47485 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10442.07164 HOMO: -7.02326 LUMO: 1.10206 factor:1 | 1 (-1.23110) | -1 | -1 |
| G: -4176.47485 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10441.94892 HOMO: -6.71305 LUMO: 0.84627 factor:1 | 1 (-1.10837) | -1 | -1 |
| G: -4176.47485 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10441.37946 HOMO: -7.27360 LUMO: 0.88165 factor:1 | 1 (-0.53892) | 1 | 1 |
| G: -4176.47485 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10441.32507 HOMO: -6.84911 LUMO: 0.59865 factor:1 | 1 (-0.48453) | -1 | -1 |
| G: -4176.47485 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10443.27395 HOMO: -6.75114 LUMO: -2.49801 factor:1 | 1 (-2.43341) | -1 | -1 |
| G: -4176.47485 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10441.47351 HOMO: -6.97156 LUMO: 0.53606 factor:1 | 1 (-0.63296) | -1 | -1 |
| G: -4176.47485 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10441.46308 HOMO: -6.54434 LUMO: 0.73199 factor:1 | 1 (-0.62254) | -1 | -1 |
| G: -4176.47485 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10441.36450 HOMO: -6.21236 LUMO: 0.99866 factor:1 | 1 (-0.52396) | -1 | -1 |
| G: -4176.47485 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10441.40812 HOMO: -6.34025 LUMO: 0.50341 factor:1 | 1 (-0.56758) | -1 | -1 |
| G: -4176.47485 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10442.50204 HOMO: -6.59876 LUMO: -0.69389 factor:1 | 1 (-1.66150) | -1 | -1 |
| G: -4176.47485 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10442.16933 HOMO: -6.54978 LUMO: -1.00682 factor:1 | 1 (-1.32879) | -1 | -1 |
| G: -4176.47485 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10441.92195 HOMO: -6.82462 LUMO: -0.98777 factor:1 | 1 (-1.08141) | -1 | -1 |
| G: -4176.47485 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10442.10329 HOMO: -6.85455 LUMO: -0.68573 factor:1 | 1 (-1.26274) | -1 | -1 |
| G: -4176.47485 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10442.73979 HOMO: -7.55388 LUMO: -0.03265 factor:1 | 1 (-1.89925) | 1 | 1 |
| G: -4176.47485 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10441.89858 HOMO: -6.77019 LUMO: -0.71838 factor:1 | 1 (-1.05803) | -1 | -1 |
| G: -4176.47485 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10442.20400 HOMO: -6.84911 LUMO: -1.25444 factor:1 | 1 (-1.36345) | -1 | -1 |
| G: -4176.47485 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10441.92350 HOMO: -6.95251 LUMO: -1.03675 factor:1 | 1 (-1.08296) | -1 | -1 |
| G: -4176.47485 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10441.87305 HOMO: -6.80829 LUMO: -0.77280 factor:1 | 1 (-1.03251) | -1 | -1 |
| G: -4176.47485 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10442.07885 HOMO: -6.94162 LUMO: -0.94151 factor:1 | 1 (-1.23831) | -1 | -1 |
| G: -4176.47485 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10442.30103 HOMO: -6.89809 LUMO: -0.90886 factor:1 | 1 (-1.46049) | -1 | -1 |
| G: -4176.47485 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10442.57217 HOMO: -6.85183 LUMO: -0.88981 factor:1 | 1 (-1.73162) | -1 | -1 |
| G: -4176.47485 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10442.10002 HOMO: -6.51985 LUMO: -0.84627 factor:1 | 1 (-1.25948) | -1 | -1 |
| G: -4176.47485 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10443.15174 HOMO: -6.83278 LUMO: -1.08029 factor:1 | 1 (-2.31120) | -1 | -1 |
| G: -4176.47485 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10440.91203 HOMO: -6.91986 LUMO: 0.66396 factor:1 | 1 (-0.07148) | -1 | -1 |
| G: -4176.47485 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10441.27688 HOMO: -6.94162 LUMO: 0.50885 factor:1 | 1 (-0.43633) | -1 | -1 |
| G: -4176.47485 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10441.17723 HOMO: -6.94435 LUMO: 0.80546 factor:1 | 1 (-0.33669) | -1 | -1 |
| G: -4176.47485 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10443.27025 HOMO: -6.74298 LUMO: -0.81634 factor:1 | 1 (-2.42970) | -1 | -1 |
| G: -4176.47485 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10441.32850 HOMO: -7.04503 LUMO: 1.15921 factor:1 | 1 (-0.48795) | -1 | -1 |
| G: -4176.47485 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10441.59256 HOMO: -6.76475 LUMO: 0.75920 factor:1 | 1 (-0.75201) | -1 | -1 |
| G: -4176.47485 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10440.89200 HOMO: -7.05047 LUMO: 0.68845 factor:1 | 1 (-0.05146) | -1 | -1 |
| G: -4176.47485 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10441.19298 HOMO: -7.12666 LUMO: 0.60681 factor:1 | 1 (-0.35244) | 1 | 1 |
| G: -4176.47485 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10443.42854 HOMO: -6.90897 LUMO: -1.22723 factor:1 | 1 (-2.58799) | -1 | -1 |
| G: -4176.47485 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10441.35552 HOMO: -7.10761 LUMO: 0.58232 factor:1 | 1 (-0.51498) | 1 | 1 |
| G: -4176.47485 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10441.06871 HOMO: -6.57427 LUMO: 0.71294 factor:1 | 1 (-0.22817) | -1 | -1 |
| G: -4176.47485 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10441.33579 HOMO: -6.22597 LUMO: 0.99322 factor:1 | 1 (-0.49525) | -1 | -1 |
| G: -4176.47485 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10443.65670 HOMO: -6.83550 LUMO: -0.77825 factor:1 | 1 (-2.81616) | -1 | -1 |
| G: -4176.47485 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10441.40861 HOMO: -7.14843 LUMO: 0.44627 factor:1 | 1 (-0.56806) | 1 | 1 |
| G: -4176.47485 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10441.23508 HOMO: -7.08040 LUMO: 0.78913 factor:1 | 1 (-0.39454) | 1 | 1 |
| G: -4176.47485 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10444.47514 HOMO: -6.81373 LUMO: -0.93879 factor:1 | 1 (-3.63460) | -1 | -1 |
| G: -4176.47485 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10444.40387 HOMO: -6.95251 LUMO: 0.22585 factor:1 | 1 (-3.56333) | -1 | -1 |
| G: -4176.47485 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10444.30197 HOMO: -7.13483 LUMO: -1.25444 factor:1 | 1 (-3.46142) | -1 | -1 |
| G: -4176.47485 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10443.68462 HOMO: -6.37835 LUMO: -1.54289 factor:1 | 1 (-2.84408) | -1 | -1 |
| G: -4176.47485 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10443.85731 HOMO: -6.53617 LUMO: -1.43948 factor:1 | 1 (-3.01676) | -1 | -1 |
| G: -4176.47485 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10442.06005 HOMO: -6.38379 LUMO: 0.16055 factor:1 | 1 (-1.21951) | -1 | -1 |
| G: -4176.47485 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10442.05025 HOMO: -6.53617 LUMO: 0.15783 factor:1 | 1 (-1.20971) | -1 | -1 |
| G: -4176.47485 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10441.71520 HOMO: -6.79740 LUMO: -0.17960 factor:1 | 1 (-0.87466) | -1 | -1 |
| G: -4176.47485 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10442.70232 HOMO: -6.26678 LUMO: -0.41361 factor:1 | 1 (-1.86178) | -1 | -1 |
| G: -4176.47485 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10442.63249 HOMO: -6.35658 LUMO: -0.24218 factor:1 | 1 (-1.79195) | -1 | -1 |
| G: -4176.47485 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10442.58063 HOMO: -6.48175 LUMO: -0.71566 factor:1 | 1 (-1.74009) | -1 | -1 |
| G: -4176.47485 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10442.70746 HOMO: -6.21508 LUMO: -0.40001 factor:1 | 1 (-1.86692) | -1 | -1 |
| G: -4176.47485 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10442.68044 HOMO: -6.51985 LUMO: -0.32654 factor:1 | 1 (-1.83990) | -1 | -1 |
| G: -4176.47485 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10442.61211 HOMO: -6.45182 LUMO: -0.66396 factor:1 | 1 (-1.77157) | -1 | -1 |
| G: -4176.47485 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10442.30634 HOMO: -6.51441 LUMO: -0.65307 factor:1 | 1 (-1.46580) | -1 | -1 |
| G: -4176.47485 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10442.10780 HOMO: -6.57971 LUMO: -0.92519 factor:1 | 1 (-1.26726) | -1 | -1 |
| G: -4176.47485 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10442.22043 HOMO: -6.67223 LUMO: -0.58232 factor:1 | 1 (-1.37989) | -1 | -1 |
| G: -4176.47485 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10442.77715 HOMO: -6.10351 LUMO: -0.45987 factor:1 | 1 (-1.93661) | -1 | -1 |
| G: -4176.47485 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10442.67454 HOMO: -6.13889 LUMO: -0.50341 factor:1 | 1 (-1.83399) | -1 | -1 |
| G: -4176.47485 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10442.95791 HOMO: -6.63141 LUMO: -0.28300 factor:1 | 1 (-2.11737) | -1 | -1 |
| G: -4176.47485 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10443.07547 HOMO: -6.37563 LUMO: -0.22858 factor:1 | 1 (-2.23493) | -1 | -1 |
| G: -4176.47485 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10441.64233 HOMO: -6.37019 LUMO: 0.11429 factor:1 | 1 (-0.80178) | -1 | -1 |
| G: -4176.47485 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10441.81708 HOMO: -6.23957 LUMO: 0.28844 factor:1 | 1 (-0.97654) | -1 | -1 |
| G: -4176.47485 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10443.26559 HOMO: -6.41372 LUMO: -0.53879 factor:1 | 1 (-2.42505) | -1 | -1 |
| G: -4176.47485 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10444.04022 HOMO: -7.06680 LUMO: 0.32654 factor:1 | 1 (-3.19968) | 1 | 1 |
| G: -4176.47485 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10443.51398 HOMO: -6.50896 LUMO: -0.73743 factor:1 | 1 (-2.67344) | -1 | -1 |
| G: -4176.47485 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10443.45033 HOMO: -6.42189 LUMO: -0.28572 factor:1 | 1 (-2.60979) | -1 | -1 |
| G: -4176.47485 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10442.58362 HOMO: -6.79740 LUMO: -0.25851 factor:1 | 1 (-1.74308) | -1 | -1 |
| G: -4176.47485 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10442.37058 HOMO: -6.32393 LUMO: 0.17960 factor:1 | 1 (-1.53004) | -1 | -1 |
| G: -4176.47485 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10442.76387 HOMO: -6.65046 LUMO: 0.03537 factor:1 | 1 (-1.92333) | -1 | -1 |
| G: -4176.47485 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10442.84047 HOMO: -6.60148 LUMO: 0.07619 factor:1 | 1 (-1.99993) | -1 | -1 |
| G: -4176.47485 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10442.59968 HOMO: -6.57971 LUMO: 0.11429 factor:1 | 1 (-1.75913) | -1 | -1 |
| G: -4176.47485 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10443.12380 HOMO: -6.88448 LUMO: -1.21907 factor:1 | 1 (-2.28325) | -1 | -1 |
| G: -4176.47485 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10441.31767 HOMO: -6.97700 LUMO: 0.36463 factor:1 | 1 (-0.47712) | -1 | -1 |
| G: -4176.47485 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10444.22858 HOMO: -6.73210 LUMO: -0.84083 factor:1 | 1 (-3.38804) | -1 | -1 |
| G: -4176.47485 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10443.31936 HOMO: -6.21236 LUMO: -0.68845 factor:1 | 1 (-2.47882) | -1 | -1 |
| G: -4176.47485 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10443.26728 HOMO: -6.35658 LUMO: -0.82995 factor:1 | 1 (-2.42674) | -1 | -1 |
| G: -4176.47485 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10443.38364 HOMO: -6.75114 LUMO: -0.94424 factor:1 | 1 (-2.54309) | -1 | -1 |
| G: -4176.47485 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10443.64884 HOMO: -6.74026 LUMO: -1.46125 factor:1 | 1 (-2.80830) | -1 | -1 |
| G: -4176.47485 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10441.99692 HOMO: -7.06952 LUMO: 0.91974 factor:1 | 1 (-1.15638) | 1 | 1 |
| G: -4176.47485 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10442.12087 HOMO: -7.08857 LUMO: 0.74559 factor:1 | 1 (-1.28032) | 1 | 1 |
| G: -4176.47485 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10441.92892 HOMO: -6.74298 LUMO: 1.03131 factor:1 | 1 (-1.08837) | -1 | -1 |
| G: -4176.47485 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10443.53186 HOMO: -6.74842 LUMO: -1.77962 factor:1 | 1 (-2.69131) | -1 | -1 |
| G: -4176.47485 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10443.60386 HOMO: -6.82462 LUMO: -1.61908 factor:1 | 1 (-2.76332) | -1 | -1 |
| G: -4176.47485 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10444.59242 HOMO: -7.17020 LUMO: -1.02043 factor:1 | 1 (-3.75188) | -1 | -1 |
| G: -4176.47485 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10443.96618 HOMO: -6.26406 LUMO: -0.96328 factor:1 | 1 (-3.12564) | -1 | -1 |
| G: -4176.47485 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10443.73730 HOMO: -6.50896 LUMO: -0.38640 factor:1 | 1 (-2.89676) | -1 | -1 |
| G: -4176.47485 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10444.53688 HOMO: -7.27632 LUMO: -1.17553 factor:1 | 1 (-3.69634) | -1 | -1 |
| G: -4176.47485 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10443.56383 HOMO: -6.54162 LUMO: -1.36873 factor:1 | 1 (-2.72329) | -1 | -1 |
| G: -4176.47485 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10443.82038 HOMO: -6.42733 LUMO: -1.15648 factor:1 | 1 (-2.97984) | -1 | -1 |
| G: -4176.47485 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10443.12023 HOMO: -6.73754 LUMO: -2.58780 factor:1 | 1 (-2.27969) | -1 | -1 |
| G: -4176.47485 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10441.18237 HOMO: -7.20285 LUMO: 0.75103 factor:1 | 1 (-0.34183) | 1 | 1 |
| G: -4176.47485 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10441.41484 HOMO: -6.98788 LUMO: 0.34831 factor:1 | 1 (-0.57430) | -1 | -1 |
| G: -4176.47485 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10441.24259 HOMO: -6.80013 LUMO: -1.11567 factor:1 | 1 (-0.40205) | -1 | -1 |
| G: -4176.47485 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10441.66619 HOMO: -6.67767 LUMO: -0.82450 factor:1 | 1 (-0.82565) | -1 | -1 |
| G: -4176.47485 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10441.64396 HOMO: -6.84911 LUMO: -0.21497 factor:1 | 1 (-0.80342) | -1 | -1 |
| G: -4176.47485 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10441.78181 HOMO: -6.23141 LUMO: 0.21769 factor:1 | 1 (-0.94127) | -1 | -1 |
| G: -4176.47485 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10441.92943 HOMO: -6.68312 LUMO: 0.16327 factor:1 | 1 (-1.08889) | -1 | -1 |
| G: -4176.47485 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10442.31861 HOMO: -7.04503 LUMO: -1.04220 factor:1 | 1 (-1.47807) | -1 | -1 |
| G: -4176.47485 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10442.16310 HOMO: -6.67495 LUMO: -0.71294 factor:1 | 1 (-1.32255) | -1 | -1 |
| G: -4176.47485 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10442.44825 HOMO: -6.70216 LUMO: -0.55239 factor:1 | 1 (-1.60770) | -1 | -1 |
| G: -4176.47485 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10442.49625 HOMO: -6.60420 LUMO: -0.71294 factor:1 | 1 (-1.65570) | -1 | -1 |
| G: -4176.47485 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10443.17403 HOMO: -7.40694 LUMO: 0.11973 factor:1 | 1 (-2.33349) | 1 | 1 |
| G: -4176.47485 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10442.30389 HOMO: -6.58788 LUMO: -0.29116 factor:1 | 1 (-1.46335) | -1 | -1 |
| G: -4176.47485 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10442.56261 HOMO: -6.63686 LUMO: -0.32654 factor:1 | 1 (-1.72207) | -1 | -1 |
| G: -4176.47485 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10442.55968 HOMO: -6.85183 LUMO: -0.95512 factor:1 | 1 (-1.71913) | -1 | -1 |
| G: -4176.47485 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10442.45546 HOMO: -6.82189 LUMO: -0.88165 factor:1 | 1 (-1.61491) | -1 | -1 |
| G: -4176.47485 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10442.59521 HOMO: -6.97428 LUMO: -1.03947 factor:1 | 1 (-1.75467) | -1 | -1 |
| G: -4176.47485 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10441.41419 HOMO: -6.51441 LUMO: -0.05714 factor:1 | 1 (-0.57364) | -1 | -1 |
| G: -4176.47485 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10442.59851 HOMO: -6.61509 LUMO: -0.77008 factor:1 | 1 (-1.75796) | -1 | -1 |
| G: -4176.47485 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10443.37602 HOMO: -7.36340 LUMO: 0.29116 factor:1 | 1 (-2.53548) | 1 | 1 |
| G: -4176.47485 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10442.55524 HOMO: -6.64230 LUMO: -0.79185 factor:1 | 1 (-1.71470) | -1 | -1 |
| G: -4176.47485 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10442.57750 HOMO: -6.56883 LUMO: -1.03403 factor:1 | 1 (-1.73696) | -1 | -1 |
| G: -4176.47485 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10442.65380 HOMO: -6.69400 LUMO: -0.77825 factor:1 | 1 (-1.81326) | -1 | -1 |
| G: -4176.47485 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10442.66969 HOMO: -6.37019 LUMO: -0.79185 factor:1 | 1 (-1.82915) | -1 | -1 |
| G: -4176.47485 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10442.17219 HOMO: -6.49808 LUMO: -0.94424 factor:1 | 1 (-1.33164) | -1 | -1 |
| G: -4176.47485 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10442.28805 HOMO: -6.91713 LUMO: -0.75376 factor:1 | 1 (-1.44751) | -1 | -1 |
| G: -4176.47485 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10443.87720 HOMO: -7.13755 LUMO: 0.41361 factor:1 | 1 (-3.03665) | 1 | 1 |
| G: -4176.47485 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10443.96670 HOMO: -7.12122 LUMO: 0.39457 factor:1 | 1 (-3.12615) | 1 | 1 |
| G: -4176.47485 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10443.33490 HOMO: -6.59332 LUMO: -0.57144 factor:1 | 1 (-2.49436) | -1 | -1 |
| G: -4176.47485 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10443.11433 HOMO: -6.62325 LUMO: -0.66940 factor:1 | 1 (-2.27378) | -1 | -1 |
| G: -4176.47485 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10442.56623 HOMO: -6.90897 LUMO: -0.08708 factor:1 | 1 (-1.72569) | -1 | -1 |
| G: -4176.47485 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10442.31398 HOMO: -6.65591 LUMO: -0.81090 factor:1 | 1 (-1.47344) | -1 | -1 |
| G: -4176.47485 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10442.20963 HOMO: -6.65318 LUMO: -0.94696 factor:1 | 1 (-1.36909) | -1 | -1 |
| G: -4176.47485 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10442.50223 HOMO: -6.96067 LUMO: -1.03675 factor:1 | 1 (-1.66169) | -1 | -1 |
| G: -4176.47485 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10442.52204 HOMO: -6.23141 LUMO: -0.66396 factor:1 | 1 (-1.68150) | -1 | -1 |
| G: -4176.47485 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10442.37867 HOMO: -6.52529 LUMO: -0.78369 factor:1 | 1 (-1.53812) | -1 | -1 |
| G: -4176.47485 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10442.65345 HOMO: -6.39468 LUMO: -0.40817 factor:1 | 1 (-1.81290) | -1 | -1 |
| G: -4176.47485 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10442.45165 HOMO: -6.76203 LUMO: -0.20409 factor:1 | 1 (-1.61110) | -1 | -1 |
| G: -4176.47485 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10442.11964 HOMO: -6.96611 LUMO: -0.90342 factor:1 | 1 (-1.27910) | -1 | -1 |
| G: -4176.47485 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10442.02669 HOMO: -6.54706 LUMO: -0.87893 factor:1 | 1 (-1.18614) | -1 | -1 |
| G: -4176.47485 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10442.39575 HOMO: -7.24367 LUMO: -0.97689 factor:1 | 1 (-1.55521) | -1 | -1 |
| G: -4176.47485 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10440.69012 HOMO: -6.61781 LUMO: 1.43404 factor:1 | -1 (0.15042) | -1 | -1 |
| G: -4176.47485 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10440.75983 HOMO: -6.17971 LUMO: 1.79867 factor:1 | -1 (0.08071) | -1 | -1 |
| G: -4176.47485 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10440.54794 HOMO: -5.73344 LUMO: 2.13609 factor:1 | -1 (0.29260) | -1 | -1 |
| G: -4176.47485 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10441.31195 HOMO: -6.72121 LUMO: 2.06807 factor:1 | 1 (-0.47141) | -1 | -1 |
| G: -4176.47485 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10441.30393 HOMO: -6.91169 LUMO: 2.02997 factor:1 | 1 (-0.46338) | -1 | -1 |
| G: -4176.47485 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10441.40934 HOMO: -7.06408 LUMO: 1.41499 factor:1 | 1 (-0.56880) | 1 | 1 |
| G: -4176.47485 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10443.60323 HOMO: -6.94162 LUMO: -0.90070 factor:1 | 1 (-2.76269) | -1 | -1 |
| G: -4176.47485 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10441.48409 HOMO: -7.09401 LUMO: 0.35103 factor:1 | 1 (-0.64355) | 1 | 1 |
| G: -4176.47485 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10441.54793 HOMO: -6.78652 LUMO: 0.91974 factor:1 | 1 (-0.70739) | -1 | -1 |
| G: -4176.47485 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10444.19737 HOMO: -6.32937 LUMO: -1.89119 factor:1 | 1 (-3.35682) | -1 | -1 |
| G: -4176.47485 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10444.46496 HOMO: -7.12666 LUMO: -1.06397 factor:1 | 1 (-3.62442) | -1 | -1 |
| G: -4176.47485 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10443.74239 HOMO: -6.38107 LUMO: -1.43132 factor:1 | 1 (-2.90185) | -1 | -1 |
| G: -4176.47485 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10444.20216 HOMO: -7.09129 LUMO: 0.08980 factor:1 | 1 (-3.36161) | 1 | 1 |
| G: -4176.47485 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10443.61482 HOMO: -6.31304 LUMO: -0.57960 factor:1 | 1 (-2.77428) | -1 | -1 |
| G: -4176.47485 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10443.89910 HOMO: -6.94435 LUMO: -0.74287 factor:1 | 1 (-3.05856) | -1 | -1 |
| G: -4176.47485 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10443.64019 HOMO: -6.35658 LUMO: -1.53472 factor:1 | 1 (-2.79964) | -1 | -1 |
| G: -4176.47485 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10443.87252 HOMO: -6.39740 LUMO: -1.48846 factor:1 | 1 (-3.03197) | -1 | -1 |
| G: -4176.47485 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10443.78756 HOMO: -7.05319 LUMO: -0.33198 factor:1 | 1 (-2.94702) | -1 | -1 |
| G: -4176.47485 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10443.80846 HOMO: -6.68040 LUMO: -0.09252 factor:1 | 1 (-2.96792) | -1 | -1 |
| G: -4176.47485 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10443.36138 HOMO: -6.35930 LUMO: -0.43266 factor:1 | 1 (-2.52084) | -1 | -1 |
| G: -4176.47485 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10443.43637 HOMO: -6.59604 LUMO: -1.45853 factor:1 | 1 (-2.59583) | -1 | -1 |
| G: -4176.47485 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10443.42317 HOMO: -6.46270 LUMO: -1.49391 factor:1 | 1 (-2.58263) | -1 | -1 |
| G: -4176.47485 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10444.06629 HOMO: -7.05863 LUMO: -1.04764 factor:1 | 1 (-3.22575) | -1 | -1 |
| G: -4176.47485 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10444.87550 HOMO: -7.14027 LUMO: -0.81634 factor:1 | 1 (-4.03496) | -1 | -1 |
| G: -4176.47485 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10443.87622 HOMO: -6.80285 LUMO: -0.74287 factor:1 | 1 (-3.03568) | -1 | -1 |
| G: -4176.47485 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10444.60916 HOMO: -6.53890 LUMO: -1.13471 factor:1 | 1 (-3.76861) | -1 | -1 |
| G: -4176.47485 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10443.83575 HOMO: -6.49808 LUMO: -1.35513 factor:1 | 1 (-2.99521) | -1 | -1 |
| G: -4176.47485 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10443.89600 HOMO: -6.75931 LUMO: -1.49663 factor:1 | 1 (-3.05546) | -1 | -1 |
| G: -4176.47485 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10443.68889 HOMO: -6.84638 LUMO: -0.77552 factor:1 | 1 (-2.84835) | -1 | -1 |
| G: -4176.47485 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10444.11799 HOMO: -6.65863 LUMO: -1.34696 factor:1 | 1 (-3.27745) | -1 | -1 |
| G: -4176.47485 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10444.22074 HOMO: -6.25590 LUMO: -2.36467 factor:1 | 1 (-3.38020) | -1 | -1 |
| G: -4176.47485 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10443.48543 HOMO: -7.24911 LUMO: 0.33470 factor:1 | 1 (-2.64489) | 1 | 1 |
| G: -4176.47485 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10442.58321 HOMO: -6.65863 LUMO: -0.75648 factor:1 | 1 (-1.74267) | -1 | -1 |
| G: -4176.47485 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10442.58155 HOMO: -6.31576 LUMO: -0.83267 factor:1 | 1 (-1.74101) | -1 | -1 |
| G: -4176.47485 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10442.72678 HOMO: -6.64774 LUMO: -0.66124 factor:1 | 1 (-1.88624) | -1 | -1 |
| G: -4176.47485 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10441.95662 HOMO: -6.75387 LUMO: -1.00138 factor:1 | 1 (-1.11607) | -1 | -1 |
| G: -4176.47485 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10442.30767 HOMO: -6.52529 LUMO: -0.68301 factor:1 | 1 (-1.46713) | -1 | -1 |
| G: -4176.47485 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10442.21774 HOMO: -6.59332 LUMO: -0.68028 factor:1 | 1 (-1.37720) | -1 | -1 |
| G: -4176.47485 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10442.25967 HOMO: -5.98650 LUMO: 0.31565 factor:1 | 1 (-1.41913) | -1 | -1 |
| G: -4176.47485 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10442.50593 HOMO: -6.59876 LUMO: 0.22585 factor:1 | 1 (-1.66539) | -1 | -1 |
| G: -4176.47485 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10442.61981 HOMO: -6.72121 LUMO: 0.10340 factor:1 | 1 (-1.77927) | -1 | -1 |
| G: -4176.47485 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10442.48278 HOMO: -6.09807 LUMO: 0.20136 factor:1 | 1 (-1.64223) | -1 | -1 |
| G: -4176.47485 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10442.49793 HOMO: -6.31576 LUMO: 0.06259 factor:1 | 1 (-1.65739) | -1 | -1 |
| G: -4176.47485 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10441.99145 HOMO: -6.35658 LUMO: -0.58232 factor:1 | 1 (-1.15091) | -1 | -1 |
| G: -4176.47485 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10442.10829 HOMO: -6.34842 LUMO: -0.55783 factor:1 | 1 (-1.26775) | -1 | -1 |
| G: -4176.47485 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10442.22416 HOMO: -6.47359 LUMO: -0.57144 factor:1 | 1 (-1.38362) | -1 | -1 |
| G: -4176.47485 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10442.71309 HOMO: -6.42189 LUMO: -0.09796 factor:1 | 1 (-1.87255) | -1 | -1 |
| G: -4176.47485 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10442.59690 HOMO: -6.35658 LUMO: -0.31293 factor:1 | 1 (-1.75636) | -1 | -1 |
| G: -4176.47485 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10443.15786 HOMO: -7.35524 LUMO: 0.10340 factor:1 | 1 (-2.31732) | 1 | 1 |
| G: -4176.47485 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10444.06164 HOMO: -7.10217 LUMO: 0.36463 factor:1 | 1 (-3.22109) | 1 | 1 |
| G: -4176.47485 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10443.18633 HOMO: -6.43549 LUMO: -0.56872 factor:1 | 1 (-2.34578) | -1 | -1 |
| G: -4176.47485 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10443.55423 HOMO: -6.50080 LUMO: -0.71294 factor:1 | 1 (-2.71368) | -1 | -1 |
| G: -4176.47485 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10443.50002 HOMO: -6.59060 LUMO: -0.57960 factor:1 | 1 (-2.65948) | -1 | -1 |
| G: -4176.47485 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10442.59453 HOMO: -6.78924 LUMO: -0.31565 factor:1 | 1 (-1.75399) | -1 | -1 |
| G: -4176.47485 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10442.47219 HOMO: -6.35658 LUMO: 0.07891 factor:1 | 1 (-1.63165) | -1 | -1 |
| G: -4176.47485 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10443.48187 HOMO: -6.74026 LUMO: -0.87621 factor:1 | 1 (-2.64133) | -1 | -1 |
| G: -4176.47485 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10441.53217 HOMO: -6.54434 LUMO: 0.81906 factor:1 | 1 (-0.69163) | -1 | -1 |
| G: -4176.47485 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10441.29296 HOMO: -6.66135 LUMO: 1.40955 factor:1 | 1 (-0.45242) | -1 | -1 |
| G: -4176.47485 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10443.23719 HOMO: -6.73754 LUMO: -2.54971 factor:1 | 1 (-2.39664) | -1 | -1 |
| G: -4176.47485 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10441.20607 HOMO: -6.65318 LUMO: 0.69389 factor:1 | 1 (-0.36553) | -1 | -1 |
| G: -4176.47485 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10441.09921 HOMO: -6.73482 LUMO: 0.62858 factor:1 | 1 (-0.25867) | -1 | -1 |
| G: -4176.47485 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10440.84348 HOMO: -6.83550 LUMO: 0.68573 factor:1 | 1 (-0.00294) | -1 | -1 |
| G: -4176.47485 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10441.32784 HOMO: -6.83278 LUMO: 0.45987 factor:1 | 1 (-0.48730) | -1 | -1 |
| G: -4176.47485 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10441.22809 HOMO: -6.78380 LUMO: 0.68301 factor:1 | 1 (-0.38754) | -1 | -1 |
| G: -4176.47485 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10441.92089 HOMO: -6.90625 LUMO: 1.36601 factor:1 | 1 (-1.08035) | -1 | -1 |
| G: -4176.47485 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10442.05480 HOMO: -6.82734 LUMO: 1.48302 factor:1 | 1 (-1.21425) | -1 | -1 |
| G: -4176.47485 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10443.25700 HOMO: -6.44094 LUMO: -0.94424 factor:1 | 1 (-2.41645) | -1 | -1 |
| G: -4176.47485 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10443.95238 HOMO: -6.91441 LUMO: 0.28844 factor:1 | 1 (-3.11184) | -1 | -1 |
| G: -4176.47485 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10443.22850 HOMO: -6.49808 LUMO: -0.51157 factor:1 | 1 (-2.38796) | -1 | -1 |
| G: -4176.47485 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10443.95535 HOMO: -7.09673 LUMO: -0.06259 factor:1 | 1 (-3.11481) | 1 | 1 |
| G: -4176.47485 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10442.20479 HOMO: -6.77019 LUMO: 0.92247 factor:1 | 1 (-1.36424) | -1 | -1 |
| G: -4176.47485 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10442.22353 HOMO: -6.75931 LUMO: 1.13744 factor:1 | 1 (-1.38299) | -1 | -1 |
| G: -4176.47485 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10441.71773 HOMO: -6.15794 LUMO: 1.12383 factor:1 | 1 (-0.87719) | -1 | -1 |
| G: -4176.47485 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10441.30863 HOMO: -6.59604 LUMO: 1.19458 factor:1 | 1 (-0.46809) | -1 | -1 |
| G: -4176.47485 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10441.26120 HOMO: -7.09401 LUMO: 0.60137 factor:1 | 1 (-0.42066) | 1 | 1 |
| G: -4176.47485 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10441.20977 HOMO: -6.34025 LUMO: 0.48164 factor:1 | 1 (-0.36923) | -1 | -1 |
| G: -4176.47485 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10443.36176 HOMO: -6.72665 LUMO: -2.47624 factor:1 | 1 (-2.52122) | -1 | -1 |
| G: -4176.47485 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10440.88299 HOMO: -6.48175 LUMO: 0.58232 factor:1 | 1 (-0.04245) | -1 | -1 |
| G: -4176.47485 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10441.49378 HOMO: -6.94162 LUMO: 0.28300 factor:1 | 1 (-0.65324) | -1 | -1 |
| G: -4176.47485 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10441.48809 HOMO: -6.65591 LUMO: 0.57144 factor:1 | 1 (-0.64755) | -1 | -1 |
| G: -4176.47485 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10443.60451 HOMO: -6.58788 LUMO: -1.03947 factor:1 | 1 (-2.76397) | -1 | -1 |
| G: -4176.47485 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10441.28509 HOMO: -7.18108 LUMO: 0.37824 factor:1 | 1 (-0.44455) | 1 | 1 |
| G: -4176.47485 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10443.60236 HOMO: -6.63958 LUMO: -1.52112 factor:1 | 1 (-2.76182) | -1 | -1 |
| G: -4176.47485 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10443.43398 HOMO: -6.12528 LUMO: -0.53606 factor:1 | 1 (-2.59344) | -1 | -1 |
| G: -4176.47485 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10442.59426 HOMO: -6.22324 LUMO: -0.87893 factor:1 | 1 (-1.75372) | -1 | -1 |
| G: -4176.47485 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10442.49802 HOMO: -6.62053 LUMO: -0.91974 factor:1 | 1 (-1.65747) | -1 | -1 |
| G: -4176.47485 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10442.63707 HOMO: -6.84366 LUMO: -0.83811 factor:1 | 1 (-1.79652) | -1 | -1 |
| G: -4176.47485 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10443.38067 HOMO: -7.26000 LUMO: 0.25851 factor:1 | 1 (-2.54013) | 1 | 1 |
| G: -4176.47485 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10441.95635 HOMO: -6.49536 LUMO: -0.63403 factor:1 | 1 (-1.11580) | -1 | -1 |
| G: -4176.47485 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10441.85272 HOMO: -6.45726 LUMO: -0.77825 factor:1 | 1 (-1.01218) | -1 | -1 |
| G: -4176.47485 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10442.20024 HOMO: -6.74570 LUMO: -0.75103 factor:1 | 1 (-1.35970) | -1 | -1 |
| G: -4176.47485 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10442.67911 HOMO: -7.20285 LUMO: 0.10612 factor:1 | 1 (-1.83856) | 1 | 1 |
| G: -4176.47485 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10442.25159 HOMO: -6.45182 LUMO: -0.56600 factor:1 | 1 (-1.41105) | -1 | -1 |
| G: -4176.47485 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10442.10691 HOMO: -6.83278 LUMO: -0.71838 factor:1 | 1 (-1.26636) | -1 | -1 |
| G: -4176.47485 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10442.36414 HOMO: -7.01510 LUMO: -1.09662 factor:1 | 1 (-1.52359) | -1 | -1 |
| G: -4176.47485 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10442.31902 HOMO: -6.48719 LUMO: 0.16871 factor:1 | 1 (-1.47848) | -1 | -1 |
| G: -4176.47485 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10443.41058 HOMO: -7.30898 LUMO: 0.26667 factor:1 | 1 (-2.57003) | 1 | 1 |
| G: -4176.47485 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10442.54495 HOMO: -6.68856 LUMO: -0.78641 factor:1 | 1 (-1.70441) | -1 | -1 |
| G: -4176.47485 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10442.74499 HOMO: -6.56883 LUMO: -1.00682 factor:1 | 1 (-1.90444) | -1 | -1 |
| G: -4176.47485 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10442.70289 HOMO: -6.41100 LUMO: -0.48980 factor:1 | 1 (-1.86235) | -1 | -1 |
| G: -4176.47485 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10442.38713 HOMO: -6.52257 LUMO: -0.59865 factor:1 | 1 (-1.54659) | -1 | -1 |
| G: -4176.47485 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10442.31167 HOMO: -6.63686 LUMO: -0.56055 factor:1 | 1 (-1.47113) | -1 | -1 |
| G: -4176.47485 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10442.57834 HOMO: -6.79740 LUMO: -0.75376 factor:1 | 1 (-1.73780) | -1 | -1 |
| G: -4176.47485 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10442.32383 HOMO: -5.89127 LUMO: 0.22313 factor:1 | 1 (-1.48329) | -1 | -1 |
| G: -4176.47485 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10441.52064 HOMO: -6.34842 LUMO: 0.11429 factor:1 | 1 (-0.68009) | -1 | -1 |
| G: -4176.47485 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10440.54813 HOMO: -6.13617 LUMO: 1.94834 factor:1 | -1 (0.29241) | -1 | -1 |
| G: -4176.47485 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10440.24241 HOMO: -6.50080 LUMO: 1.74153 factor:1 | -1 (0.59813) | -1 | -1 |
| G: -4176.47485 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10440.84503 HOMO: -6.33481 LUMO: 1.68438 factor:1 | 1 (-0.00449) | -1 | -1 |
| G: -4176.47485 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10441.61179 HOMO: -6.53073 LUMO: 1.95106 factor:1 | 1 (-0.77125) | -1 | -1 |
| G: -4176.47485 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10441.59068 HOMO: -6.46270 LUMO: 1.89935 factor:1 | 1 (-0.75014) | -1 | -1 |
| G: -4176.47485 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10440.96743 HOMO: -5.87222 LUMO: 1.91568 factor:1 | 1 (-0.12689) | -1 | -1 |
| G: -4176.47485 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10440.93205 HOMO: -6.07630 LUMO: 1.81500 factor:1 | 1 (-0.09151) | -1 | -1 |
| G: -4176.47485 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10441.03578 HOMO: -6.20964 LUMO: 1.81500 factor:1 | 1 (-0.19524) | -1 | -1 |
| G: -4176.47485 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10441.08177 HOMO: -6.15522 LUMO: 1.90752 factor:1 | 1 (-0.24123) | -1 | -1 |
| G: -4176.47485 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10440.96852 HOMO: -6.11984 LUMO: 1.95378 factor:1 | 1 (-0.12798) | -1 | -1 |
| G: -4176.47485 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10441.16996 HOMO: -6.58516 LUMO: 2.04358 factor:1 | 1 (-0.32942) | -1 | -1 |
| G: -4176.47485 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10443.39297 HOMO: -7.37156 LUMO: 0.24490 factor:1 | 1 (-2.55243) | 1 | 1 |
| G: -4176.47485 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10442.45831 HOMO: -6.36474 LUMO: -0.90070 factor:1 | 1 (-1.61777) | -1 | -1 |
| G: -4176.47485 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10442.62545 HOMO: -6.43549 LUMO: -0.40817 factor:1 | 1 (-1.78490) | -1 | -1 |
| G: -4176.47485 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10443.87940 HOMO: -7.32258 LUMO: 0.29388 factor:1 | 1 (-3.03886) | 1 | 1 |
| G: -4176.47485 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10443.34257 HOMO: -6.41372 LUMO: -0.20409 factor:1 | 1 (-2.50203) | -1 | -1 |
| G: -4176.47485 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10444.07083 HOMO: -7.18381 LUMO: 0.42722 factor:1 | 1 (-3.23029) | 1 | 1 |
| G: -4176.47485 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10443.32369 HOMO: -6.53890 LUMO: -0.54151 factor:1 | 1 (-2.48315) | -1 | -1 |
| G: -4176.47485 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10441.73855 HOMO: -6.61509 LUMO: 0.08708 factor:1 | 1 (-0.89800) | -1 | -1 |
| G: -4176.47485 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10440.51836 HOMO: -6.78108 LUMO: 2.03541 factor:1 | -1 (0.32218) | -1 | -1 |
| G: -4176.47485 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10440.10831 HOMO: -6.50896 LUMO: 1.53472 factor:1 | -1 (0.73223) | -1 | -1 |
| G: -4176.47485 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10440.00279 HOMO: -6.65591 LUMO: 1.80411 factor:1 | -1 (0.83776) | -1 | -1 |
| G: -4176.47485 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10440.44652 HOMO: -6.64502 LUMO: 1.52112 factor:1 | -1 (0.39402) | -1 | -1 |
| G: -4176.47485 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10440.34135 HOMO: -6.72938 LUMO: 1.48030 factor:1 | -1 (0.49919) | -1 | -1 |
| G: -4176.47485 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10440.88201 HOMO: -6.16882 LUMO: 1.96466 factor:1 | 1 (-0.04147) | -1 | -1 |
| G: -4176.47485 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10440.36758 HOMO: -6.22597 LUMO: 1.43132 factor:1 | -1 (0.47296) | -1 | -1 |
| G: -4176.47485 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10441.64867 HOMO: -6.57699 LUMO: 2.05718 factor:1 | 1 (-0.80812) | -1 | -1 |
| G: -4176.47485 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10441.58559 HOMO: -6.52529 LUMO: 1.89663 factor:1 | 1 (-0.74505) | -1 | -1 |
| G: -4176.47485 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10441.57345 HOMO: -6.30760 LUMO: 1.88031 factor:1 | 1 (-0.73291) | -1 | -1 |
| G: -4176.47485 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10440.88667 HOMO: -6.14977 LUMO: 1.92657 factor:1 | 1 (-0.04612) | -1 | -1 |
| G: -4176.47485 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10440.87192 HOMO: -6.20964 LUMO: 1.83949 factor:1 | 1 (-0.03137) | -1 | -1 |
| G: -4176.47485 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10441.19924 HOMO: -6.31848 LUMO: 1.91296 factor:1 | 1 (-0.35870) | -1 | -1 |
| G: -4176.47485 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10441.70641 HOMO: -5.80691 LUMO: 2.19868 factor:1 | 1 (-0.86587) | -1 | -1 |
| G: -4176.47485 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10441.87792 HOMO: -6.00827 LUMO: 2.15514 factor:1 | 1 (-1.03738) | -1 | -1 |
| G: -4176.47485 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10441.94206 HOMO: -6.51713 LUMO: 2.08711 factor:1 | 1 (-1.10152) | -1 | -1 |
| G: -4176.47485 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10441.23464 HOMO: -6.32937 LUMO: 2.11705 factor:1 | 1 (-0.39410) | -1 | -1 |
| G: -4176.47485 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10441.66276 HOMO: -6.26678 LUMO: 1.95922 factor:1 | 1 (-0.82222) | -1 | -1 |
| G: -4176.47485 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10442.66251 HOMO: -6.43005 LUMO: 2.56603 factor:1 | 1 (-1.82197) | -1 | -1 |
| G: -4176.47485 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10442.78529 HOMO: -6.41644 LUMO: 2.68304 factor:1 | 1 (-1.94474) | -1 | -1 |
| G: -4176.47485 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10442.61263 HOMO: -5.97834 LUMO: 2.02997 factor:1 | 1 (-1.77209) | -1 | -1 |
| G: -4176.47485 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10441.06095 HOMO: -6.14161 LUMO: 1.77690 factor:1 | 1 (-0.22041) | -1 | -1 |
| G: -4176.47485 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10441.22447 HOMO: -6.21508 LUMO: 1.80411 factor:1 | 1 (-0.38393) | -1 | -1 |
| G: -4176.47485 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10442.83650 HOMO: -6.46270 LUMO: 2.34562 factor:1 | 1 (-1.99596) | -1 | -1 |
| G: -4176.47485 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10441.14958 HOMO: -6.39195 LUMO: -0.75920 factor:1 | 1 (-0.30904) | -1 | -1 |
| G: -4176.47485 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10441.67852 HOMO: -7.08584 LUMO: -1.14016 factor:1 | 1 (-0.83797) | -1 | -1 |
| G: -4176.47485 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10441.98723 HOMO: -6.70216 LUMO: -0.65035 factor:1 | 1 (-1.14669) | -1 | -1 |
| G: -4176.47485 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10442.41314 HOMO: -6.79468 LUMO: -0.83811 factor:1 | 1 (-1.57260) | -1 | -1 |
| G: -4176.47485 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10441.84263 HOMO: -6.99877 LUMO: -0.79729 factor:1 | 1 (-1.00209) | -1 | -1 |
| G: -4176.47485 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10441.98214 HOMO: -7.08040 LUMO: -0.85444 factor:1 | 1 (-1.14160) | -1 | -1 |
| G: -4176.47485 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10442.73884 HOMO: -7.39333 LUMO: 0.12789 factor:1 | 1 (-1.89829) | 1 | 1 |
| G: -4176.47485 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10443.12665 HOMO: -7.05047 LUMO: 0.13878 factor:1 | 1 (-2.28611) | -1 | -1 |
| G: -4176.47485 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10442.19828 HOMO: -6.90897 LUMO: -0.77552 factor:1 | 1 (-1.35774) | -1 | -1 |
| G: -4176.47485 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10442.96488 HOMO: -7.25456 LUMO: 0.05170 factor:1 | 1 (-2.12434) | 1 | 1 |
| G: -4176.47485 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10442.34422 HOMO: -6.84638 LUMO: -0.84355 factor:1 | 1 (-1.50367) | -1 | -1 |
| G: -4176.47485 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10442.06778 HOMO: -6.78108 LUMO: -0.81634 factor:1 | 1 (-1.22723) | -1 | -1 |
| G: -4176.47485 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10442.45192 HOMO: -6.74570 LUMO: -0.77280 factor:1 | 1 (-1.61138) | -1 | -1 |
| G: -4176.47485 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10442.12723 HOMO: -7.28177 LUMO: -1.68438 factor:1 | 1 (-1.28669) | -1 | -1 |
| G: -4176.47485 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10442.16753 HOMO: -7.22190 LUMO: -1.63540 factor:1 | 1 (-1.32699) | -1 | -1 |
| G: -4176.47485 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10442.36223 HOMO: -7.15932 LUMO: -1.57554 factor:1 | 1 (-1.52169) | -1 | -1 |
| G: -4176.47485 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10443.13909 HOMO: -6.57971 LUMO: -0.93063 factor:1 | 1 (-2.29855) | -1 | -1 |
| G: -4176.47485 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10440.90155 HOMO: -6.88176 LUMO: 0.58232 factor:1 | 1 (-0.06101) | -1 | -1 |
| G: -4176.47485 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10441.12243 HOMO: -6.85727 LUMO: 0.51430 factor:1 | 1 (-0.28188) | -1 | -1 |
| G: -4176.47485 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10441.28129 HOMO: -6.83550 LUMO: 0.87893 factor:1 | 1 (-0.44074) | -1 | -1 |
| G: -4176.47485 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10441.91262 HOMO: -7.06680 LUMO: 0.87621 factor:1 | 1 (-1.07207) | 1 | 1 |
| G: -4176.47485 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10441.71098 HOMO: -6.52257 LUMO: 0.81362 factor:1 | 1 (-0.87044) | -1 | -1 |
| G: -4176.47485 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10441.97833 HOMO: -6.95523 LUMO: 1.17009 factor:1 | 1 (-1.13779) | -1 | -1 |
| G: -4176.47485 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10441.84976 HOMO: -7.21374 LUMO: 0.97145 factor:1 | 1 (-1.00922) | 1 | 1 |
| G: -4176.47485 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10443.52870 HOMO: -6.81373 LUMO: -1.54561 factor:1 | 1 (-2.68816) | -1 | -1 |
| G: -4176.47485 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10443.54655 HOMO: -6.86543 LUMO: -1.52656 factor:1 | 1 (-2.70601) | -1 | -1 |
| G: -4176.47485 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10443.25770 HOMO: -6.90081 LUMO: -0.78097 factor:1 | 1 (-2.41716) | -1 | -1 |
| G: -4176.47485 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10443.18510 HOMO: -6.64502 LUMO: -0.82723 factor:1 | 1 (-2.34456) | -1 | -1 |
| G: -4176.47485 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10443.27144 HOMO: -6.65591 LUMO: -0.82178 factor:1 | 1 (-2.43090) | -1 | -1 |
| G: -4176.47485 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10442.93620 HOMO: -6.79468 LUMO: -1.46397 factor:1 | 1 (-2.09566) | -1 | -1 |
| G: -4176.47485 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10440.82451 HOMO: -7.25728 LUMO: 0.73743 factor:1 | -1 (0.01603) | 1 | -1 |
| G: -4176.47485 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10441.10879 HOMO: -7.00149 LUMO: 1.30070 factor:1 | 1 (-0.26825) | -1 | -1 |
| G: -4176.47485 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10440.81319 HOMO: -7.07768 LUMO: 0.78097 factor:1 | -1 (0.02735) | 1 | -1 |
| G: -4176.47485 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10441.32297 HOMO: -6.86271 LUMO: 0.86260 factor:1 | 1 (-0.48243) | -1 | -1 |
| G: -4176.47485 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10440.99810 HOMO: -6.94707 LUMO: 0.39729 factor:1 | 1 (-0.15755) | -1 | -1 |
| G: -4176.47485 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10441.40121 HOMO: -6.79740 LUMO: 0.67484 factor:1 | 1 (-0.56066) | -1 | -1 |
| G: -4176.47485 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10443.14927 HOMO: -6.91986 LUMO: -1.14288 factor:1 | 1 (-2.30872) | -1 | -1 |
| G: -4176.47485 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10441.00996 HOMO: -6.31576 LUMO: 1.01771 factor:1 | 1 (-0.16942) | -1 | -1 |
| G: -4176.47485 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10441.34959 HOMO: -6.81645 LUMO: 0.81362 factor:1 | 1 (-0.50904) | -1 | -1 |
| G: -4176.47485 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10443.13237 HOMO: -6.92258 LUMO: -0.99594 factor:1 | 1 (-2.29182) | -1 | -1 |
| G: -4176.47485 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10441.60744 HOMO: -6.81373 LUMO: 0.61770 factor:1 | 1 (-0.76690) | -1 | -1 |
| G: -4176.47485 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10441.22507 HOMO: -7.18653 LUMO: 1.19186 factor:1 | 1 (-0.38452) | 1 | 1 |
| G: -4176.47485 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10440.94495 HOMO: -7.00693 LUMO: 0.45715 factor:1 | 1 (-0.10441) | -1 | -1 |
| G: -4176.47485 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10441.21424 HOMO: -7.11306 LUMO: 0.53334 factor:1 | 1 (-0.37369) | 1 | 1 |
| G: -4176.47485 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10443.58851 HOMO: -6.63414 LUMO: -1.64357 factor:1 | 1 (-2.74797) | -1 | -1 |
| G: -4176.47485 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10443.29123 HOMO: -6.22052 LUMO: -0.74015 factor:1 | 1 (-2.45068) | -1 | -1 |
| G: -4176.47485 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10443.41844 HOMO: -6.81101 LUMO: -0.50069 factor:1 | 1 (-2.57790) | -1 | -1 |
| G: -4176.47485 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10443.37757 HOMO: -6.71849 LUMO: -0.51974 factor:1 | 1 (-2.53703) | -1 | -1 |
| G: -4176.47485 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10443.53937 HOMO: -6.72121 LUMO: -1.77690 factor:1 | 1 (-2.69883) | -1 | -1 |
| G: -4176.47485 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10443.72906 HOMO: -6.94162 LUMO: -1.78779 factor:1 | 1 (-2.88852) | -1 | -1 |
| G: -4176.47485 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10441.98228 HOMO: -6.91169 LUMO: 0.88981 factor:1 | 1 (-1.14174) | -1 | -1 |
| G: -4176.47485 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10441.96192 HOMO: -6.97428 LUMO: 0.70750 factor:1 | 1 (-1.12138) | -1 | -1 |
| G: -4176.47485 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10441.90568 HOMO: -6.74842 LUMO: 1.15921 factor:1 | 1 (-1.06514) | -1 | -1 |
| G: -4176.47485 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10444.60518 HOMO: -7.25183 LUMO: -0.99594 factor:1 | 1 (-3.76464) | -1 | -1 |
| G: -4176.47485 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10443.98022 HOMO: -6.43821 LUMO: -1.00410 factor:1 | 1 (-3.13968) | -1 | -1 |
| G: -4176.47485 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10443.24584 HOMO: -6.52257 LUMO: -0.68573 factor:1 | 1 (-2.40530) | -1 | -1 |
| G: -4176.47485 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10443.61033 HOMO: -6.60148 LUMO: -0.52518 factor:1 | 1 (-2.76979) | -1 | -1 |
| G: -4176.47485 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10443.52889 HOMO: -6.07086 LUMO: -1.39594 factor:1 | 1 (-2.68835) | -1 | -1 |
| G: -4176.47485 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10443.93244 HOMO: -6.78108 LUMO: -1.54833 factor:1 | 1 (-3.09189) | -1 | -1 |
| G: -4176.47485 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10443.47060 HOMO: -6.73482 LUMO: -1.01498 factor:1 | 1 (-2.63006) | -1 | -1 |
| G: -4176.47485 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10441.57865 HOMO: -6.85183 LUMO: 1.06669 factor:1 | 1 (-0.73811) | -1 | -1 |
| G: -4176.47485 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10441.19135 HOMO: -6.98516 LUMO: 1.43948 factor:1 | 1 (-0.35081) | -1 | -1 |
| G: -4176.47485 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10441.61321 HOMO: -6.94162 LUMO: 0.79185 factor:1 | 1 (-0.77267) | -1 | -1 |
| G: -4176.47485 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10442.22623 HOMO: -6.67495 LUMO: -1.06669 factor:1 | 1 (-1.38569) | -1 | -1 |
| G: -4176.47485 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10442.18481 HOMO: -6.88720 LUMO: -1.00682 factor:1 | 1 (-1.34427) | -1 | -1 |
| G: -4176.47485 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10442.28669 HOMO: -6.85999 LUMO: -0.78097 factor:1 | 1 (-1.44615) | -1 | -1 |
| G: -4176.47485 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10442.10595 HOMO: -6.51713 LUMO: -0.89798 factor:1 | 1 (-1.26541) | -1 | -1 |
| G: -4176.47485 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10442.07515 HOMO: -6.63141 LUMO: -0.91430 factor:1 | 1 (-1.23461) | -1 | -1 |
| G: -4176.47485 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10442.33809 HOMO: -6.63414 LUMO: 0.04354 factor:1 | 1 (-1.49755) | -1 | -1 |
| G: -4176.47485 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10442.04495 HOMO: -6.65046 LUMO: -0.73743 factor:1 | 1 (-1.20440) | -1 | -1 |
| G: -4176.47485 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10442.11134 HOMO: -6.73754 LUMO: -0.71838 factor:1 | 1 (-1.27080) | -1 | -1 |
| G: -4176.47485 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10442.36669 HOMO: -6.65863 LUMO: -0.60137 factor:1 | 1 (-1.52615) | -1 | -1 |
| G: -4176.47485 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10442.87799 HOMO: -6.61509 LUMO: -0.47892 factor:1 | 1 (-2.03745) | -1 | -1 |
| G: -4176.47485 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10443.05337 HOMO: -6.82189 LUMO: -0.64763 factor:1 | 1 (-2.21283) | -1 | -1 |
| G: -4176.47485 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10442.96540 HOMO: -6.56883 LUMO: -0.51974 factor:1 | 1 (-2.12486) | -1 | -1 |
| G: -4176.47485 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10443.25275 HOMO: -6.97428 LUMO: -0.95512 factor:1 | 1 (-2.41221) | -1 | -1 |
| G: -4176.47485 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10442.48139 HOMO: -6.70489 LUMO: -0.04082 factor:1 | 1 (-1.64085) | -1 | -1 |
| G: -4176.47485 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10442.49279 HOMO: -6.74026 LUMO: 0.02177 factor:1 | 1 (-1.65225) | -1 | -1 |
| G: -4176.47485 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10443.25076 HOMO: -6.50080 LUMO: -0.89525 factor:1 | 1 (-2.41022) | -1 | -1 |
| G: -4176.47485 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10443.25705 HOMO: -6.46815 LUMO: -0.61226 factor:1 | 1 (-2.41651) | -1 | -1 |
| G: -4176.47485 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10443.17098 HOMO: -6.57971 LUMO: -0.64219 factor:1 | 1 (-2.33044) | -1 | -1 |
| G: -4176.47485 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10444.01293 HOMO: -7.17836 LUMO: 0.37280 factor:1 | 1 (-3.17239) | 1 | 1 |
| G: -4176.47485 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10442.49366 HOMO: -6.67223 LUMO: 0.12245 factor:1 | 1 (-1.65312) | -1 | -1 |
| G: -4176.47485 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10442.50433 HOMO: -6.55250 LUMO: 0.22858 factor:1 | 1 (-1.66379) | -1 | -1 |
| G: -4176.47485 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10442.18446 HOMO: -6.97156 LUMO: -1.12927 factor:1 | 1 (-1.34392) | -1 | -1 |
| G: -4176.47485 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10442.20772 HOMO: -6.78924 LUMO: -0.84900 factor:1 | 1 (-1.36718) | -1 | -1 |
| G: -4176.47485 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10442.42449 HOMO: -6.65046 LUMO: -0.65307 factor:1 | 1 (-1.58395) | -1 | -1 |
| G: -4176.47485 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10443.05993 HOMO: -7.41782 LUMO: 0.08980 factor:1 | 1 (-2.21939) | 1 | 1 |
| G: -4176.47485 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10442.52906 HOMO: -6.56339 LUMO: -0.68573 factor:1 | 1 (-1.68852) | -1 | -1 |
| G: -4176.47485 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10442.30326 HOMO: -6.31032 LUMO: -0.31837 factor:1 | 1 (-1.46272) | -1 | -1 |
| G: -4176.47485 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10442.59913 HOMO: -6.72938 LUMO: -0.45987 factor:1 | 1 (-1.75859) | -1 | -1 |
| G: -4176.47485 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10442.56770 HOMO: -6.59876 LUMO: -1.03131 factor:1 | 1 (-1.72716) | -1 | -1 |
| G: -4176.47485 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10443.54122 HOMO: -7.29265 LUMO: 0.29660 factor:1 | 1 (-2.70068) | 1 | 1 |
| G: -4176.47485 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10442.74765 HOMO: -6.42189 LUMO: -0.51157 factor:1 | 1 (-1.90711) | -1 | -1 |
| G: -4176.47485 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10442.76150 HOMO: -6.27767 LUMO: -0.52790 factor:1 | 1 (-1.92096) | -1 | -1 |
| G: -4176.47485 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10442.96809 HOMO: -6.41644 LUMO: -0.44627 factor:1 | 1 (-2.12755) | -1 | -1 |
| G: -4176.47485 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10443.14257 HOMO: -6.23413 LUMO: -0.52790 factor:1 | 1 (-2.30203) | -1 | -1 |
| G: -4176.47485 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10442.99299 HOMO: -6.63414 LUMO: -0.44082 factor:1 | 1 (-2.15245) | -1 | -1 |
| G: -4176.47485 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10443.76051 HOMO: -7.03142 LUMO: 0.47076 factor:1 | 1 (-2.91997) | -1 | -1 |
| G: -4176.47485 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10442.32275 HOMO: -6.62053 LUMO: -0.14422 factor:1 | 1 (-1.48220) | -1 | -1 |
| G: -4176.47485 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10440.31351 HOMO: -6.22324 LUMO: 1.96194 factor:1 | -1 (0.52703) | -1 | -1 |
| G: -4176.47485 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10440.27746 HOMO: -6.17971 LUMO: 1.71704 factor:1 | -1 (0.56309) | -1 | -1 |
| G: -4176.47485 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10440.69665 HOMO: -6.70761 LUMO: 1.68711 factor:1 | -1 (0.14389) | -1 | -1 |
| G: -4176.47485 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10441.01108 HOMO: -6.52801 LUMO: 1.56193 factor:1 | 1 (-0.17053) | -1 | -1 |
| G: -4176.47485 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10441.00335 HOMO: -6.55794 LUMO: 1.52384 factor:1 | 1 (-0.16281) | -1 | -1 |
| G: -4176.47485 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10440.95426 HOMO: -6.47359 LUMO: 1.82316 factor:1 | 1 (-0.11372) | -1 | -1 |
| G: -4176.47485 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10440.95135 HOMO: -6.65863 LUMO: 1.83133 factor:1 | 1 (-0.11080) | -1 | -1 |
| G: -4176.47485 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10441.10093 HOMO: -6.46270 LUMO: 1.90208 factor:1 | 1 (-0.26039) | -1 | -1 |
| G: -4176.47485 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10441.19331 HOMO: -6.41917 LUMO: 2.03269 factor:1 | 1 (-0.35277) | -1 | -1 |
| G: -4176.47485 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10441.38033 HOMO: -6.48992 LUMO: 1.87486 factor:1 | 1 (-0.53979) | -1 | -1 |
| G: -4176.47485 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10441.51658 HOMO: -6.51985 LUMO: 1.69527 factor:1 | 1 (-0.67604) | -1 | -1 |
| G: -4176.47485 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10441.17064 HOMO: -6.36202 LUMO: 2.05718 factor:1 | 1 (-0.33010) | -1 | -1 |
| G: -4176.47485 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10440.88269 HOMO: -5.96474 LUMO: 1.88575 factor:1 | 1 (-0.04215) | -1 | -1 |
| G: -4176.47485 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10441.28207 HOMO: -6.56339 LUMO: 2.04630 factor:1 | 1 (-0.44153) | -1 | -1 |
| G: -4176.47485 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10441.30833 HOMO: -6.43277 LUMO: 1.98371 factor:1 | 1 (-0.46779) | -1 | -1 |
| G: -4176.47485 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10441.13611 HOMO: -6.53345 LUMO: 2.06262 factor:1 | 1 (-0.29557) | -1 | -1 |
| G: -4176.47485 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10441.63487 HOMO: -5.81779 LUMO: 2.11432 factor:1 | 1 (-0.79433) | -1 | -1 |
| G: -4176.47485 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10441.76687 HOMO: -5.91848 LUMO: 1.86942 factor:1 | 1 (-0.92633) | -1 | -1 |
| G: -4176.47485 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10441.81011 HOMO: -6.48447 LUMO: 1.70343 factor:1 | 1 (-0.96957) | -1 | -1 |
| G: -4176.47485 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10442.30890 HOMO: -6.29671 LUMO: -0.89525 factor:1 | 1 (-1.46835) | -1 | -1 |
| G: -4176.47485 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10442.49913 HOMO: -6.63414 LUMO: -0.76192 factor:1 | 1 (-1.65859) | -1 | -1 |
| G: -4176.47485 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10442.53622 HOMO: -6.56883 LUMO: -0.86260 factor:1 | 1 (-1.69568) | -1 | -1 |
| G: -4176.47485 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10442.71560 HOMO: -6.93074 LUMO: -0.27483 factor:1 | 1 (-1.87505) | -1 | -1 |
| G: -4176.47485 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10442.90001 HOMO: -6.85999 LUMO: -0.01905 factor:1 | 1 (-2.05947) | -1 | -1 |
| G: -4176.47485 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10442.66341 HOMO: -6.26406 LUMO: 0.21769 factor:1 | 1 (-1.82286) | -1 | -1 |
| G: -4176.47485 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10443.19427 HOMO: -6.62325 LUMO: 0.31293 factor:1 | 1 (-2.35373) | -1 | -1 |
| G: -4176.47485 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10443.12663 HOMO: -6.59604 LUMO: 0.19592 factor:1 | 1 (-2.28608) | -1 | -1 |
| G: -4176.47485 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10442.59372 HOMO: -6.43277 LUMO: -0.27756 factor:1 | 1 (-1.75318) | -1 | -1 |
| G: -4176.47485 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10442.51113 HOMO: -6.54978 LUMO: -0.46531 factor:1 | 1 (-1.67059) | -1 | -1 |
| G: -4176.47485 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10442.58569 HOMO: -6.65046 LUMO: -0.15783 factor:1 | 1 (-1.74515) | -1 | -1 |
| G: -4176.47485 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10443.87203 HOMO: -7.28721 LUMO: 0.23946 factor:1 | 1 (-3.03148) | 1 | 1 |
| G: -4176.47485 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10443.43809 HOMO: -6.71849 LUMO: -0.56600 factor:1 | 1 (-2.59754) | -1 | -1 |
| G: -4176.47485 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10443.35487 HOMO: -6.85183 LUMO: -0.84355 factor:1 | 1 (-2.51433) | -1 | -1 |
| G: -4176.47485 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10443.28143 HOMO: -6.53345 LUMO: -0.84627 factor:1 | 1 (-2.44089) | -1 | -1 |
| G: -4176.47485 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10443.18320 HOMO: -6.60148 LUMO: -0.63130 factor:1 | 1 (-2.34266) | -1 | -1 |
| G: -4176.47485 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10443.33471 HOMO: -6.36202 LUMO: -0.60137 factor:1 | 1 (-2.49417) | -1 | -1 |
| G: -4176.47485 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10442.76439 HOMO: -6.28855 LUMO: -0.52790 factor:1 | 1 (-1.92384) | -1 | -1 |
| G: -4176.47485 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10443.42780 HOMO: -7.07224 LUMO: 0.41906 factor:1 | 1 (-2.58726) | 1 | 1 |
| G: -4176.47485 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10442.97394 HOMO: -6.36202 LUMO: -0.24218 factor:1 | 1 (-2.13340) | -1 | -1 |
| G: -4176.47485 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10441.74679 HOMO: -6.43549 LUMO: 0.14150 factor:1 | 1 (-0.90625) | -1 | -1 |
| G: -4176.47485 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10442.70757 HOMO: -6.76747 LUMO: -0.40545 factor:1 | 1 (-1.86703) | -1 | -1 |
| G: -4176.47485 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10442.67070 HOMO: -6.15249 LUMO: -0.51157 factor:1 | 1 (-1.83016) | -1 | -1 |
| G: -4176.47485 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10442.90839 HOMO: -6.33753 LUMO: -0.02993 factor:1 | 1 (-2.06785) | -1 | -1 |
| G: -4176.47485 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10442.76314 HOMO: -6.49808 LUMO: -0.83811 factor:1 | 1 (-1.92259) | -1 | -1 |
| G: -4176.47485 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10443.06175 HOMO: -6.64502 LUMO: -0.46259 factor:1 | 1 (-2.22121) | -1 | -1 |
| G: -4176.47485 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10442.39456 HOMO: -6.34570 LUMO: 0.22041 factor:1 | 1 (-1.55402) | -1 | -1 |
| G: -4176.47485 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10442.55676 HOMO: -6.63414 LUMO: -0.13606 factor:1 | 1 (-1.71622) | -1 | -1 |
| G: -4176.47485 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10443.31863 HOMO: -6.59604 LUMO: -0.79729 factor:1 | 1 (-2.47809) | -1 | -1 |
| G: -4176.47485 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10444.05981 HOMO: -7.09401 LUMO: 0.31837 factor:1 | 1 (-3.21927) | 1 | 1 |
| G: -4176.47485 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10443.39109 HOMO: -6.48719 LUMO: -0.31021 factor:1 | 1 (-2.55055) | -1 | -1 |
| G: -4176.47485 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10443.79262 HOMO: -7.11306 LUMO: 0.39729 factor:1 | 1 (-2.95208) | 1 | 1 |
| G: -4176.47485 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10443.72435 HOMO: -6.95251 LUMO: 0.41089 factor:1 | 1 (-2.88381) | -1 | -1 |
| G: -4176.47485 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10443.37052 HOMO: -6.61509 LUMO: -0.41906 factor:1 | 1 (-2.52998) | -1 | -1 |
| G: -4176.47485 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10443.01389 HOMO: -6.25318 LUMO: -0.47348 factor:1 | 1 (-2.17335) | -1 | -1 |
| G: -4176.47485 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10442.43731 HOMO: -6.77019 LUMO: -0.10340 factor:1 | 1 (-1.59676) | -1 | -1 |
| G: -4176.47485 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10443.70209 HOMO: -6.54706 LUMO: -0.46259 factor:1 | 1 (-2.86155) | -1 | -1 |
| G: -4176.47485 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10443.79837 HOMO: -6.34297 LUMO: -0.50341 factor:1 | 1 (-2.95782) | -1 | -1 |
| G: -4176.47485 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10443.61485 HOMO: -6.20692 LUMO: -0.51974 factor:1 | 1 (-2.77431) | -1 | -1 |
| G: -4176.47485 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10444.50311 HOMO: -7.03686 LUMO: 0.46804 factor:1 | 1 (-3.66257) | -1 | -1 |
| G: -4176.47485 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10442.76909 HOMO: -6.47087 LUMO: 0.22585 factor:1 | 1 (-1.92855) | -1 | -1 |
| G: -4176.47485 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10442.75413 HOMO: -6.41917 LUMO: 0.19320 factor:1 | 1 (-1.91359) | -1 | -1 |
| G: -4176.47485 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10442.66120 HOMO: -6.61237 LUMO: -0.04354 factor:1 | 1 (-1.82066) | -1 | -1 |
| G: -4176.47485 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10442.62477 HOMO: -6.56339 LUMO: 0.36735 factor:1 | 1 (-1.78422) | -1 | -1 |
| G: -4176.47485 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10439.34188 HOMO: -6.54978 LUMO: 1.12655 factor:1 | -1 (1.49867) | -1 | -1 |
| G: -4176.47485 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10439.44283 HOMO: -6.43277 LUMO: 1.17553 factor:1 | -1 (1.39771) | -1 | -1 |
| G: -4176.47485 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10439.56074 HOMO: -6.29944 LUMO: 1.40955 factor:1 | -1 (1.27981) | -1 | -1 |
| G: -4176.47485 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10439.11934 HOMO: -6.74842 LUMO: 0.74015 factor:1 | -1 (1.72120) | -1 | -1 |
| G: -4176.47485 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10441.21541 HOMO: -6.15522 LUMO: 1.94289 factor:1 | 1 (-0.37486) | -1 | -1 |
| G: -4176.47485 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10441.05984 HOMO: -6.20147 LUMO: 1.40139 factor:1 | 1 (-0.21930) | -1 | -1 |
| G: -4176.47485 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10441.21247 HOMO: -6.41100 LUMO: 1.40139 factor:1 | 1 (-0.37193) | -1 | -1 |
| G: -4176.47485 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10441.49868 HOMO: -6.74570 LUMO: 1.80956 factor:1 | 1 (-0.65813) | -1 | -1 |
| G: -4176.47485 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10441.13296 HOMO: -6.60148 LUMO: -1.04764 factor:1 | 1 (-0.29241) | -1 | -1 |
| G: -4176.47485 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10441.47408 HOMO: -6.82734 LUMO: -0.83267 factor:1 | 1 (-0.63354) | -1 | -1 |
| G: -4176.47485 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10441.35780 HOMO: -7.01782 LUMO: -0.32382 factor:1 | 1 (-0.51726) | -1 | -1 |
| G: -4176.47485 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10441.58320 HOMO: -6.54434 LUMO: 0.11157 factor:1 | 1 (-0.74265) | -1 | -1 |
| G: -4176.47485 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10441.64317 HOMO: -6.53617 LUMO: 0.32926 factor:1 | 1 (-0.80263) | -1 | -1 |
| G: -4176.47485 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10442.54917 HOMO: -6.62597 LUMO: -0.60137 factor:1 | 1 (-1.70863) | -1 | -1 |
| G: -4176.47485 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10442.37921 HOMO: -6.60965 LUMO: -0.75376 factor:1 | 1 (-1.53867) | -1 | -1 |
| G: -4176.47485 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10441.33949 HOMO: -6.29399 LUMO: 0.06803 factor:1 | 1 (-0.49895) | -1 | -1 |
| G: -4176.47485 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10442.50982 HOMO: -6.60692 LUMO: -0.47076 factor:1 | 1 (-1.66928) | -1 | -1 |
| G: -4176.47485 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10443.41869 HOMO: -7.33891 LUMO: 0.39184 factor:1 | 1 (-2.57814) | 1 | 1 |
| G: -4176.47485 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10439.88561 HOMO: -6.60692 LUMO: 1.46125 factor:1 | -1 (0.95493) | -1 | -1 |
| G: -4176.47485 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10439.94602 HOMO: -6.21780 LUMO: 2.09256 factor:1 | -1 (0.89452) | -1 | -1 |
| G: -4176.47485 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10440.06314 HOMO: -6.28311 LUMO: 1.80411 factor:1 | -1 (0.77740) | -1 | -1 |
| G: -4176.47485 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10440.20279 HOMO: -6.51168 LUMO: 1.84765 factor:1 | -1 (0.63775) | -1 | -1 |
| G: -4176.47485 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10440.09130 HOMO: -6.66951 LUMO: 2.01636 factor:1 | -1 (0.74924) | -1 | -1 |
| G: -4176.47485 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10440.50848 HOMO: -6.75387 LUMO: 1.73881 factor:1 | -1 (0.33206) | -1 | -1 |
| G: -4176.47485 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10440.23735 HOMO: -6.77291 LUMO: 1.89935 factor:1 | -1 (0.60319) | -1 | -1 |
| G: -4176.47485 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10441.10925 HOMO: -6.36474 LUMO: 1.61091 factor:1 | 1 (-0.26871) | -1 | -1 |
| G: -4176.47485 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10441.16662 HOMO: -6.60420 LUMO: 1.40955 factor:1 | 1 (-0.32607) | -1 | -1 |
| G: -4176.47485 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10441.19486 HOMO: -6.81645 LUMO: 1.59731 factor:1 | 1 (-0.35432) | -1 | -1 |
| G: -4176.47485 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10440.49069 HOMO: -5.90215 LUMO: 2.12249 factor:1 | -1 (0.34986) | -1 | -1 |
| G: -4176.47485 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10440.71322 HOMO: -6.26950 LUMO: 1.62996 factor:1 | -1 (0.12732) | -1 | -1 |
| G: -4176.47485 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10440.85317 HOMO: -6.41100 LUMO: 1.80684 factor:1 | 1 (-0.01263) | -1 | -1 |
| G: -4176.47485 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10441.57462 HOMO: -6.64230 LUMO: 2.23405 factor:1 | 1 (-0.73408) | -1 | -1 |
| G: -4176.47485 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10440.40072 HOMO: -6.66951 LUMO: 2.21501 factor:1 | -1 (0.43982) | -1 | -1 |
| G: -4176.47485 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10440.76157 HOMO: -6.90897 LUMO: 2.00004 factor:1 | -1 (0.07897) | -1 | -1 |
| G: -4176.47485 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10440.87276 HOMO: -6.61781 LUMO: 1.42043 factor:1 | 1 (-0.03222) | -1 | -1 |
| G: -4176.47485 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10440.99483 HOMO: -6.56611 LUMO: 1.60003 factor:1 | 1 (-0.15429) | -1 | -1 |
| G: -4176.47485 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10441.04528 HOMO: -6.70489 LUMO: 1.78779 factor:1 | 1 (-0.20474) | -1 | -1 |
| G: -4176.47485 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10440.99050 HOMO: -6.46815 LUMO: 1.59459 factor:1 | 1 (-0.14996) | -1 | -1 |
| G: -4176.47485 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10440.62027 HOMO: -6.31304 LUMO: 1.36873 factor:1 | -1 (0.22028) | -1 | -1 |
| G: -4176.47485 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10440.38810 HOMO: -6.22597 LUMO: 1.54833 factor:1 | -1 (0.45244) | -1 | -1 |
| G: -4176.47485 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10440.42508 HOMO: -5.63004 LUMO: 1.96466 factor:1 | -1 (0.41546) | -1 | -1 |
| G: -4176.47485 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10442.11795 HOMO: -7.02598 LUMO: 1.79323 factor:1 | 1 (-1.27741) | -1 | -1 |
| G: -4176.47485 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10442.06133 HOMO: -6.78924 LUMO: 2.10888 factor:1 | 1 (-1.22078) | -1 | -1 |
| G: -4176.47485 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10441.64061 HOMO: -6.13345 LUMO: 2.07351 factor:1 | 1 (-0.80007) | -1 | -1 |
| G: -4176.47485 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10442.31638 HOMO: -6.46270 LUMO: -0.37552 factor:1 | 1 (-1.47584) | -1 | -1 |
| G: -4176.47485 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10442.10016 HOMO: -6.51985 LUMO: -0.49525 factor:1 | 1 (-1.25962) | -1 | -1 |
| G: -4176.47485 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10440.96678 HOMO: -6.60965 LUMO: 1.90480 factor:1 | 1 (-0.12623) | -1 | -1 |
| G: -4176.47485 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10441.20346 HOMO: -6.51168 LUMO: 1.92112 factor:1 | 1 (-0.36292) | -1 | -1 |
| G: -4176.47485 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10440.99799 HOMO: -6.71305 LUMO: 1.91024 factor:1 | 1 (-0.15745) | -1 | -1 |
| G: -4176.47485 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10441.24616 HOMO: -6.86815 LUMO: 2.02997 factor:1 | 1 (-0.40561) | -1 | -1 |
| G: -4176.47485 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10441.01886 HOMO: -6.69944 LUMO: 1.95106 factor:1 | 1 (-0.17832) | -1 | -1 |
| G: -4176.47485 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10440.88620 HOMO: -6.45182 LUMO: 1.66806 factor:1 | 1 (-0.04566) | -1 | -1 |
| G: -4176.47485 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10441.30855 HOMO: -6.44638 LUMO: 2.16058 factor:1 | 1 (-0.46801) | -1 | -1 |
| G: -4176.47485 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10441.43133 HOMO: -6.65591 LUMO: 1.95106 factor:1 | 1 (-0.59079) | -1 | -1 |
| G: -4176.47485 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10440.76323 HOMO: -6.35114 LUMO: 1.42316 factor:1 | -1 (0.07731) | -1 | -1 |
| G: -4176.47485 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10441.28188 HOMO: -6.48719 LUMO: 1.59187 factor:1 | 1 (-0.44134) | -1 | -1 |
| G: -4176.47485 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10442.10571 HOMO: -7.05591 LUMO: 1.61908 factor:1 | 1 (-1.26517) | -1 | -1 |
| G: -4176.47485 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10442.10712 HOMO: -6.92258 LUMO: 1.87214 factor:1 | 1 (-1.26658) | -1 | -1 |
| G: -4176.47485 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10441.66173 HOMO: -5.85861 LUMO: 2.11705 factor:1 | 1 (-0.82119) | -1 | -1 |
| G: -4176.47485 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10441.84127 HOMO: -6.27767 LUMO: 1.75513 factor:1 | 1 (-1.00073) | -1 | -1 |
| G: -4176.47485 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10440.77172 HOMO: -6.16882 LUMO: 1.73881 factor:1 | -1 (0.06882) | -1 | -1 |
| G: -4176.47485 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10440.67289 HOMO: -6.62053 LUMO: 1.39594 factor:1 | -1 (0.16765) | -1 | -1 |
| G: -4176.47485 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10440.59937 HOMO: -5.46405 LUMO: 1.68166 factor:1 | -1 (0.24117) | -1 | -1 |
| G: -4176.47485 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10440.86860 HOMO: -6.39740 LUMO: 1.68711 factor:1 | 1 (-0.02805) | -1 | -1 |
| G: -4176.47485 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10441.29369 HOMO: -6.99333 LUMO: 2.08439 factor:1 | 1 (-0.45315) | -1 | -1 |
| G: -4176.47485 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10440.95924 HOMO: -6.16882 LUMO: 1.71976 factor:1 | 1 (-0.11870) | -1 | -1 |
| G: -4176.47485 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10442.16971 HOMO: -7.19741 LUMO: 2.24766 factor:1 | 1 (-1.32917) | 1 | 1 |
| G: -4176.47485 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10441.33364 HOMO: -6.77291 LUMO: 2.17691 factor:1 | 1 (-0.49310) | -1 | -1 |
| G: -4176.47485 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10441.35174 HOMO: -6.29944 LUMO: 2.16603 factor:1 | 1 (-0.51119) | -1 | -1 |
| G: -4176.47485 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10441.00972 HOMO: -6.10079 LUMO: 1.83949 factor:1 | 1 (-0.16917) | -1 | -1 |
| G: -4176.47485 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10441.29378 HOMO: -6.63686 LUMO: 2.05990 factor:1 | 1 (-0.45323) | -1 | -1 |
| G: -4176.47485 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10441.49359 HOMO: -6.91713 LUMO: 1.87486 factor:1 | 1 (-0.65305) | -1 | -1 |
| G: -4176.47485 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10441.20455 HOMO: -6.63958 LUMO: 1.79323 factor:1 | 1 (-0.36401) | -1 | -1 |
| G: -4176.47485 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10441.26156 HOMO: -6.61781 LUMO: 1.70071 factor:1 | 1 (-0.42101) | -1 | -1 |
| G: -4176.47485 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10441.33742 HOMO: -6.20420 LUMO: 1.82861 factor:1 | 1 (-0.49688) | -1 | -1 |
| G: -4176.47485 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10443.71578 HOMO: -6.47903 LUMO: -2.16875 factor:1 | 1 (-2.87524) | -1 | -1 |
| G: -4176.47485 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10440.26352 HOMO: -6.53073 LUMO: 2.18235 factor:1 | -1 (0.57702) | -1 | -1 |
| G: -4176.47485 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10440.56032 HOMO: -7.01782 LUMO: 1.72520 factor:1 | -1 (0.28022) | -1 | -1 |
| G: -4176.47485 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10441.06378 HOMO: -6.66135 LUMO: -0.75648 factor:1 | 1 (-0.22324) | -1 | -1 |
| G: -4176.47485 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10442.13393 HOMO: -7.56749 LUMO: 0.22585 factor:1 | 1 (-1.29338) | 1 | 1 |
| G: -4176.47485 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10441.39035 HOMO: -6.45182 LUMO: -0.71294 factor:1 | 1 (-0.54981) | -1 | -1 |
| G: -4176.47485 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10442.13221 HOMO: -6.31032 LUMO: -0.34286 factor:1 | 1 (-1.29167) | -1 | -1 |
| G: -4176.47485 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10440.29898 HOMO: -6.41917 LUMO: 2.04085 factor:1 | -1 (0.54156) | -1 | -1 |
| G: -4176.47485 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10440.10203 HOMO: -6.61781 LUMO: 1.98915 factor:1 | -1 (0.73852) | -1 | -1 |
| G: -4176.47485 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10440.77940 HOMO: -5.86405 LUMO: 1.57282 factor:1 | -1 (0.06114) | -1 | -1 |
| G: -4176.47485 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10440.68917 HOMO: -6.44094 LUMO: 1.80956 factor:1 | -1 (0.15138) | -1 | -1 |
| G: -4176.47485 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10440.23403 HOMO: -6.59060 LUMO: 2.08167 factor:1 | -1 (0.60651) | -1 | -1 |
| G: -4176.47485 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10439.91797 HOMO: -6.20147 LUMO: 1.69799 factor:1 | -1 (0.92257) | -1 | -1 |
| G: -4176.47485 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10442.95846 HOMO: -6.50352 LUMO: -0.41361 factor:1 | 1 (-2.11792) | -1 | -1 |
| G: -4176.47485 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10442.76714 HOMO: -6.10896 LUMO: -0.55783 factor:1 | 1 (-1.92659) | -1 | -1 |
| G: -4176.47485 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10443.04309 HOMO: -6.74842 LUMO: -0.56872 factor:1 | 1 (-2.20254) | -1 | -1 |
| G: -4176.47485 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10442.40971 HOMO: -6.59060 LUMO: -0.22041 factor:1 | 1 (-1.56917) | -1 | -1 |
| G: -4176.47485 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10443.40375 HOMO: -6.22052 LUMO: -0.60137 factor:1 | 1 (-2.56320) | -1 | -1 |
| G: -4176.47485 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10442.71364 HOMO: -6.65863 LUMO: 0.07891 factor:1 | 1 (-1.87310) | -1 | -1 |
| G: -4176.47485 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10441.41685 HOMO: -6.57427 LUMO: 1.71160 factor:1 | 1 (-0.57631) | -1 | -1 |
| G: -4176.47485 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10441.58023 HOMO: -5.84773 LUMO: 1.99459 factor:1 | 1 (-0.73969) | -1 | -1 |
| G: -4176.47485 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10441.78924 HOMO: -6.02188 LUMO: 1.91296 factor:1 | 1 (-0.94870) | -1 | -1 |
| G: -4176.47485 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10441.85354 HOMO: -6.17698 LUMO: 2.00004 factor:1 | 1 (-1.01300) | -1 | -1 |
| G: -4176.47485 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10441.80124 HOMO: -6.02732 LUMO: 1.90752 factor:1 | 1 (-0.96070) | -1 | -1 |
| G: -4176.47485 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10442.13999 HOMO: -6.68584 LUMO: -0.50885 factor:1 | 1 (-1.29945) | -1 | -1 |
| G: -4176.47485 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10442.07463 HOMO: -6.61781 LUMO: -0.73471 factor:1 | 1 (-1.23409) | -1 | -1 |
| G: -4176.47485 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10442.07003 HOMO: -6.66407 LUMO: -0.79729 factor:1 | 1 (-1.22949) | -1 | -1 |
| G: -4176.47485 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10441.96220 HOMO: -6.56339 LUMO: 0.23130 factor:1 | 1 (-1.12165) | -1 | -1 |
| G: -4176.47485 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10442.26318 HOMO: -6.76747 LUMO: 0.08980 factor:1 | 1 (-1.42264) | -1 | -1 |
| G: -4176.47485 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10441.80105 HOMO: -6.70489 LUMO: -0.53334 factor:1 | 1 (-0.96051) | -1 | -1 |
| G: -4176.47485 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10442.61527 HOMO: -7.28993 LUMO: 0.10885 factor:1 | 1 (-1.77473) | 1 | 1 |
| G: -4176.47485 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10442.73005 HOMO: -6.22052 LUMO: 0.51974 factor:1 | 1 (-1.88950) | -1 | -1 |
| G: -4176.47485 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10443.23751 HOMO: -6.81645 LUMO: 0.25307 factor:1 | 1 (-2.39697) | -1 | -1 |
| G: -4176.47485 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10442.91699 HOMO: -6.80285 LUMO: 0.02721 factor:1 | 1 (-2.07645) | -1 | -1 |
| G: -4176.47485 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10442.66357 HOMO: -6.51441 LUMO: 0.08163 factor:1 | 1 (-1.82303) | -1 | -1 |
| G: -4176.47485 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10441.78755 HOMO: -6.73482 LUMO: -0.77008 factor:1 | 1 (-0.94701) | -1 | -1 |
| G: -4176.47485 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10442.10467 HOMO: -6.29127 LUMO: -0.44355 factor:1 | 1 (-1.26413) | -1 | -1 |
| G: -4176.47485 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10443.06170 HOMO: -6.72938 LUMO: -0.64763 factor:1 | 1 (-2.22116) | -1 | -1 |
| G: -4176.47485 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10442.71435 HOMO: -6.49264 LUMO: -0.74559 factor:1 | 1 (-1.87380) | -1 | -1 |
| G: -4176.47485 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10442.79544 HOMO: -6.67223 LUMO: -0.55239 factor:1 | 1 (-1.95489) | -1 | -1 |
| G: -4176.47485 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10442.38332 HOMO: -6.33481 LUMO: 0.33198 factor:1 | 1 (-1.54278) | -1 | -1 |
| G: -4176.47485 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10441.91090 HOMO: -6.76475 LUMO: -0.25307 factor:1 | 1 (-1.07036) | -1 | -1 |
| G: -4176.47485 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10442.26939 HOMO: -6.65318 LUMO: 0.03810 factor:1 | 1 (-1.42884) | -1 | -1 |
| G: -4176.47485 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10442.24394 HOMO: -6.09263 LUMO: 0.21497 factor:1 | 1 (-1.40340) | -1 | -1 |
| G: -4176.47485 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10443.10755 HOMO: -6.32120 LUMO: -0.85444 factor:1 | 1 (-2.26701) | -1 | -1 |
| G: -4176.47485 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10443.28755 HOMO: -6.57155 LUMO: -0.67484 factor:1 | 1 (-2.44701) | -1 | -1 |
| G: -4176.47485 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10443.15340 HOMO: -6.53345 LUMO: -0.78913 factor:1 | 1 (-2.31286) | -1 | -1 |
| G: -4176.47485 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10443.92025 HOMO: -7.07768 LUMO: 0.28844 factor:1 | 1 (-3.07970) | 1 | 1 |
| G: -4176.47485 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10442.51263 HOMO: -6.75114 LUMO: 0.18776 factor:1 | 1 (-1.67209) | -1 | -1 |
| G: -4176.47485 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10442.40618 HOMO: -6.77019 LUMO: -0.12245 factor:1 | 1 (-1.56563) | -1 | -1 |
| G: -4176.47485 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10441.60992 HOMO: -6.43549 LUMO: 0.16327 factor:1 | 1 (-0.76937) | -1 | -1 |
| G: -4176.47485 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10442.12682 HOMO: -6.69400 LUMO: -0.16327 factor:1 | 1 (-1.28628) | -1 | -1 |
| G: -4176.47485 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10441.97052 HOMO: -6.38651 LUMO: -0.61770 factor:1 | 1 (-1.12998) | -1 | -1 |
| G: -4176.47485 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10442.18130 HOMO: -6.34297 LUMO: -0.33198 factor:1 | 1 (-1.34076) | -1 | -1 |
| G: -4176.47485 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10442.98091 HOMO: -7.51578 LUMO: 0.02177 factor:1 | 1 (-2.14037) | 1 | 1 |
| G: -4176.47485 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10442.31970 HOMO: -6.47359 LUMO: -0.22585 factor:1 | 1 (-1.47916) | -1 | -1 |
| G: -4176.47485 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10442.43453 HOMO: -6.68040 LUMO: -0.47076 factor:1 | 1 (-1.59399) | -1 | -1 |
| G: -4176.47485 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10442.03017 HOMO: -6.75659 LUMO: -0.57688 factor:1 | 1 (-1.18963) | -1 | -1 |
| G: -4176.47485 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10441.87863 HOMO: -6.73754 LUMO: -0.61226 factor:1 | 1 (-1.03809) | -1 | -1 |
| G: -4176.47485 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10442.74458 HOMO: -7.37429 LUMO: 0.31293 factor:1 | 1 (-1.90404) | 1 | 1 |
| G: -4176.47485 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10443.17430 HOMO: -6.23413 LUMO: -0.90886 factor:1 | 1 (-2.33376) | -1 | -1 |
| G: -4176.47485 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10443.26431 HOMO: -6.51985 LUMO: -0.68028 factor:1 | 1 (-2.42377) | -1 | -1 |
| G: -4176.47485 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10443.30407 HOMO: -6.52257 LUMO: -0.77280 factor:1 | 1 (-2.46353) | -1 | -1 |
| G: -4176.47485 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10444.29876 HOMO: -7.29537 LUMO: 0.31837 factor:1 | 1 (-3.45821) | 1 | 1 |
| G: -4176.47485 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10441.74693 HOMO: -6.08447 LUMO: 0.25851 factor:1 | 1 (-0.90638) | -1 | -1 |
| G: -4176.47485 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10441.86666 HOMO: -6.20964 LUMO: 0.13606 factor:1 | 1 (-1.02611) | -1 | -1 |
| G: -4176.47485 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10442.44637 HOMO: -6.49808 LUMO: -0.14150 factor:1 | 1 (-1.60583) | -1 | -1 |
| G: -4176.47485 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10443.94240 HOMO: -7.10761 LUMO: 0.28028 factor:1 | 1 (-3.10185) | 1 | 1 |
| G: -4176.47485 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10443.06619 HOMO: -6.60965 LUMO: -0.62858 factor:1 | 1 (-2.22565) | -1 | -1 |
| G: -4176.47485 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10443.38168 HOMO: -6.40012 LUMO: -0.26939 factor:1 | 1 (-2.54114) | -1 | -1 |
| G: -4176.47485 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10443.35398 HOMO: -6.65318 LUMO: -0.73199 factor:1 | 1 (-2.51343) | -1 | -1 |
| G: -4176.47485 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10443.13541 HOMO: -6.51441 LUMO: -0.44899 factor:1 | 1 (-2.29487) | -1 | -1 |
| G: -4176.47485 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10443.02129 HOMO: -6.28583 LUMO: -0.48708 factor:1 | 1 (-2.18075) | -1 | -1 |
| G: -4176.47485 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10443.74930 HOMO: -6.96884 LUMO: 0.19864 factor:1 | 1 (-2.90876) | -1 | -1 |
| G: -4176.47485 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10442.70338 HOMO: -6.89809 LUMO: 0.34558 factor:1 | 1 (-1.86284) | -1 | -1 |
| G: -4176.47485 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10442.62670 HOMO: -6.67495 LUMO: -0.15510 factor:1 | 1 (-1.78616) | -1 | -1 |
| G: -4176.47485 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10443.38127 HOMO: -7.34980 LUMO: 0.19864 factor:1 | 1 (-2.54073) | 1 | 1 |
| G: -4176.47485 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10442.61396 HOMO: -6.71305 LUMO: -0.81634 factor:1 | 1 (-1.77342) | -1 | -1 |
| G: -4176.47485 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10442.56346 HOMO: -6.39468 LUMO: -0.47076 factor:1 | 1 (-1.72292) | -1 | -1 |
| G: -4176.47485 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10441.14327 HOMO: -6.31304 LUMO: 1.39594 factor:1 | 1 (-0.30273) | -1 | -1 |
| G: -4176.47485 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10441.03524 HOMO: -6.57155 LUMO: 1.55105 factor:1 | 1 (-0.19470) | -1 | -1 |
| G: -4176.47485 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10440.98789 HOMO: -6.68312 LUMO: 1.69255 factor:1 | 1 (-0.14735) | -1 | -1 |
| G: -4176.47485 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10441.45800 HOMO: -6.61509 LUMO: 1.73881 factor:1 | 1 (-0.61745) | -1 | -1 |
| G: -4176.47485 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10441.62521 HOMO: -6.17971 LUMO: 1.90208 factor:1 | 1 (-0.78467) | -1 | -1 |
| G: -4176.47485 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10441.90916 HOMO: -6.53073 LUMO: 1.73337 factor:1 | 1 (-1.06862) | -1 | -1 |
| G: -4176.47485 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10441.57770 HOMO: -5.91303 LUMO: 1.90480 factor:1 | 1 (-0.73716) | -1 | -1 |
| G: -4176.47485 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10441.82815 HOMO: -6.42733 LUMO: 1.80139 factor:1 | 1 (-0.98761) | -1 | -1 |
| G: -4176.47485 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10442.03515 HOMO: -6.78924 LUMO: 2.31569 factor:1 | 1 (-1.19461) | -1 | -1 |
| G: -4176.47485 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10441.86078 HOMO: -6.04093 LUMO: 1.91568 factor:1 | 1 (-1.02024) | -1 | -1 |
| G: -4176.47485 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10442.88915 HOMO: -6.90081 LUMO: 2.36739 factor:1 | 1 (-2.04861) | -1 | -1 |
| G: -4176.47485 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10442.83799 HOMO: -6.60965 LUMO: 2.18507 factor:1 | 1 (-1.99745) | -1 | -1 |
| G: -4176.47485 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10442.80934 HOMO: -6.75387 LUMO: 2.48712 factor:1 | 1 (-1.96880) | -1 | -1 |
| G: -4176.47485 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10441.38001 HOMO: -6.56883 LUMO: 1.71432 factor:1 | 1 (-0.53947) | -1 | -1 |
| G: -4176.47485 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10441.44083 HOMO: -6.41644 LUMO: 1.72792 factor:1 | 1 (-0.60028) | -1 | -1 |
| G: -4176.47485 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10442.58738 HOMO: -6.92530 LUMO: 2.54426 factor:1 | 1 (-1.74683) | -1 | -1 |
| G: -4176.47485 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10442.52207 HOMO: -6.41644 LUMO: 2.70209 factor:1 | 1 (-1.68153) | -1 | -1 |
| G: -4176.47485 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10439.82406 HOMO: -6.29671 LUMO: 2.14698 factor:1 | -1 (1.01648) | -1 | -1 |
| G: -4176.47485 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10439.92180 HOMO: -6.29127 LUMO: 1.87486 factor:1 | -1 (0.91874) | -1 | -1 |
| G: -4176.47485 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10441.46989 HOMO: -6.75931 LUMO: 2.78917 factor:1 | 1 (-0.62934) | -1 | -1 |
| G: -4176.47485 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10441.04427 HOMO: -6.40828 LUMO: 1.86942 factor:1 | 1 (-0.20373) | -1 | -1 |
| G: -4176.47485 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10440.93679 HOMO: -6.45726 LUMO: 1.97010 factor:1 | 1 (-0.09625) | -1 | -1 |
| G: -4176.47485 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10440.78636 HOMO: -6.43277 LUMO: 1.22723 factor:1 | -1 (0.05418) | -1 | -1 |
| G: -4176.47485 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10440.95317 HOMO: -6.63414 LUMO: 1.62452 factor:1 | 1 (-0.11263) | -1 | -1 |
| G: -4176.47485 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10441.52197 HOMO: -6.54162 LUMO: 2.16058 factor:1 | 1 (-0.68143) | -1 | -1 |
| G: -4176.47485 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10441.07949 HOMO: -6.40284 LUMO: 1.88575 factor:1 | 1 (-0.23894) | -1 | -1 |
| G: -4176.47485 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10441.11135 HOMO: -6.20964 LUMO: 1.84221 factor:1 | 1 (-0.27081) | -1 | -1 |
| G: -4176.47485 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10440.78449 HOMO: -6.58516 LUMO: 1.69799 factor:1 | -1 (0.05606) | -1 | -1 |
| G: -4176.47485 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10441.84750 HOMO: -6.44094 LUMO: 2.05446 factor:1 | 1 (-1.00696) | -1 | -1 |
| G: -4176.47485 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10441.24779 HOMO: -6.61509 LUMO: 2.16058 factor:1 | 1 (-0.40725) | -1 | -1 |
| G: -4176.47485 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10441.97512 HOMO: -6.65591 LUMO: 1.69527 factor:1 | 1 (-1.13458) | -1 | -1 |
| G: -4176.47485 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10440.28410 HOMO: -5.55112 LUMO: 1.80411 factor:1 | -1 (0.55645) | -1 | -1 |
| G: -4176.47485 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10442.23047 HOMO: -6.68312 LUMO: 2.38100 factor:1 | 1 (-1.38993) | -1 | -1 |
| G: -4176.47485 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10441.50681 HOMO: -6.51168 LUMO: 2.14698 factor:1 | 1 (-0.66627) | -1 | -1 |
| G: -4176.47485 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10441.00027 HOMO: -6.04637 LUMO: 1.48302 factor:1 | 1 (-0.15973) | -1 | -1 |
| G: -4176.47485 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10442.19722 HOMO: -6.81645 LUMO: -0.74287 factor:1 | 1 (-1.35668) | -1 | -1 |
| G: -4176.47485 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10442.21034 HOMO: -6.96884 LUMO: -0.97961 factor:1 | 1 (-1.36979) | -1 | -1 |
| G: -4176.47485 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10441.69917 HOMO: -6.45998 LUMO: 0.09796 factor:1 | 1 (-0.85863) | -1 | -1 |
| G: -4176.47485 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10441.81621 HOMO: -6.44638 LUMO: 0.09524 factor:1 | 1 (-0.97566) | -1 | -1 |
| G: -4176.47485 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10442.52969 HOMO: -6.16338 LUMO: -0.54151 factor:1 | 1 (-1.68915) | -1 | -1 |
| G: -4176.47485 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10442.87639 HOMO: -6.35930 LUMO: -0.47892 factor:1 | 1 (-2.03585) | -1 | -1 |
| G: -4176.47485 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10442.66830 HOMO: -6.65318 LUMO: -0.00272 factor:1 | 1 (-1.82776) | -1 | -1 |
| G: -4176.47485 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10442.88216 HOMO: -6.50080 LUMO: 0.14694 factor:1 | 1 (-2.04162) | -1 | -1 |
| G: -4176.47485 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10440.27683 HOMO: -6.60420 LUMO: 0.94968 factor:1 | -1 (0.56371) | -1 | -1 |
| G: -4176.47485 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10442.07246 HOMO: -6.60148 LUMO: -0.77552 factor:1 | 1 (-1.23191) | -1 | -1 |
| G: -4176.47485 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10442.26231 HOMO: -6.81645 LUMO: -1.05580 factor:1 | 1 (-1.42177) | -1 | -1 |
| G: -4176.47485 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10442.28593 HOMO: -6.57971 LUMO: -0.82178 factor:1 | 1 (-1.44539) | -1 | -1 |
| G: -4176.47485 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10442.27325 HOMO: -6.09263 LUMO: -0.45171 factor:1 | 1 (-1.43271) | -1 | -1 |
| G: -4176.47485 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10442.47235 HOMO: -6.74298 LUMO: -0.61770 factor:1 | 1 (-1.63181) | -1 | -1 |
| G: -4176.47485 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10440.38764 HOMO: -6.72393 LUMO: 1.21091 factor:1 | -1 (0.45291) | -1 | -1 |
| G: -4176.47485 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10440.20061 HOMO: -6.30488 LUMO: 1.70071 factor:1 | -1 (0.63993) | -1 | -1 |
| G: -4176.47485 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10440.48875 HOMO: -6.38107 LUMO: 1.55649 factor:1 | -1 (0.35179) | -1 | -1 |
| G: -4176.47485 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10440.51662 HOMO: -6.17154 LUMO: 1.46669 factor:1 | -1 (0.32392) | -1 | -1 |
| G: -4176.47485 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10441.11007 HOMO: -6.86543 LUMO: 1.98643 factor:1 | 1 (-0.26953) | -1 | -1 |
| G: -4176.47485 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10441.27222 HOMO: -6.69944 LUMO: 1.65173 factor:1 | 1 (-0.43168) | -1 | -1 |
| G: -4176.47485 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10441.22319 HOMO: -6.77836 LUMO: 2.16331 factor:1 | 1 (-0.38265) | -1 | -1 |
| G: -4176.47485 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10441.92244 HOMO: -6.42189 LUMO: 2.36467 factor:1 | 1 (-1.08190) | -1 | -1 |
| G: -4176.47485 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10442.14759 HOMO: -7.00965 LUMO: 2.04358 factor:1 | 1 (-1.30704) | -1 | -1 |
| G: -4176.47485 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10441.79485 HOMO: -6.36746 LUMO: 2.13881 factor:1 | 1 (-0.95430) | -1 | -1 |
| G: -4176.47485 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10441.16542 HOMO: -6.37835 LUMO: 1.89935 factor:1 | 1 (-0.32488) | -1 | -1 |
| G: -4176.47485 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10441.27875 HOMO: -7.03959 LUMO: 1.27349 factor:1 | 1 (-0.43821) | -1 | -1 |
| G: -4176.47485 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10442.37186 HOMO: -6.67495 LUMO: -0.89253 factor:1 | 1 (-1.53132) | -1 | -1 |
| G: -4176.47485 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10442.48087 HOMO: -6.71849 LUMO: -0.97961 factor:1 | 1 (-1.64033) | -1 | -1 |
| G: -4176.47485 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10441.06438 HOMO: -6.47903 LUMO: 0.01633 factor:1 | 1 (-0.22384) | -1 | -1 |
| G: -4176.47485 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10441.20659 HOMO: -6.38379 LUMO: 0.01088 factor:1 | 1 (-0.36605) | -1 | -1 |
| G: -4176.47485 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10442.74988 HOMO: -6.49536 LUMO: -0.55239 factor:1 | 1 (-1.90934) | -1 | -1 |
| G: -4176.47485 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10442.87146 HOMO: -6.53345 LUMO: -0.53879 factor:1 | 1 (-2.03092) | -1 | -1 |
| G: -4176.47485 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10440.49817 HOMO: -6.16610 LUMO: 2.15514 factor:1 | -1 (0.34237) | -1 | -1 |
| G: -4176.47485 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10440.77736 HOMO: -6.35114 LUMO: 1.98643 factor:1 | -1 (0.06318) | -1 | -1 |
| G: -4176.47485 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10441.42112 HOMO: -6.43277 LUMO: 2.16058 factor:1 | 1 (-0.58058) | -1 | -1 |
| G: -4176.47485 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10441.41846 HOMO: -6.89809 LUMO: 2.20684 factor:1 | 1 (-0.57792) | -1 | -1 |
| G: -4176.47485 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10441.09783 HOMO: -6.54434 LUMO: 1.93473 factor:1 | 1 (-0.25728) | -1 | -1 |
| G: -4176.47485 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10441.27622 HOMO: -6.72938 LUMO: 2.03269 factor:1 | 1 (-0.43568) | -1 | -1 |
| G: -4176.47485 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10441.19478 HOMO: -6.90353 LUMO: 2.19868 factor:1 | 1 (-0.35424) | -1 | -1 |
| G: -4176.47485 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10441.18346 HOMO: -6.41372 LUMO: 2.02453 factor:1 | 1 (-0.34292) | -1 | -1 |
| G: -4176.47485 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10441.54377 HOMO: -6.46543 LUMO: 1.90752 factor:1 | 1 (-0.70322) | -1 | -1 |
| G: -4176.47485 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10441.65016 HOMO: -6.55522 LUMO: 2.11977 factor:1 | 1 (-0.80962) | -1 | -1 |
| G: -4176.47485 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10440.56176 HOMO: -6.28855 LUMO: 2.02181 factor:1 | -1 (0.27878) | -1 | -1 |
| G: -4176.47485 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10440.69774 HOMO: -6.45726 LUMO: 1.52112 factor:1 | -1 (0.14281) | -1 | -1 |
| G: -4176.47485 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10441.44262 HOMO: -6.37291 LUMO: 2.11705 factor:1 | 1 (-0.60208) | -1 | -1 |
| G: -4176.47485 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10442.25937 HOMO: -6.88448 LUMO: 2.24494 factor:1 | 1 (-1.41883) | -1 | -1 |
| G: -4176.47485 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10442.42702 HOMO: -6.86271 LUMO: 2.41637 factor:1 | 1 (-1.58648) | -1 | -1 |
| G: -4176.47485 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10442.31513 HOMO: -6.69400 LUMO: 2.34562 factor:1 | 1 (-1.47459) | -1 | -1 |
| G: -4176.47485 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10442.23785 HOMO: -6.18243 LUMO: 2.53882 factor:1 | 1 (-1.39730) | -1 | -1 |
| G: -4176.47485 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10442.43837 HOMO: -6.61237 LUMO: 2.54154 factor:1 | 1 (-1.59783) | -1 | -1 |
| G: -4176.47485 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10442.22732 HOMO: -6.69672 LUMO: 2.16331 factor:1 | 1 (-1.38677) | -1 | -1 |
| G: -4176.47485 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10442.16946 HOMO: -6.33481 LUMO: 2.34018 factor:1 | 1 (-1.32892) | -1 | -1 |
| G: -4176.47485 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10442.05632 HOMO: -5.99739 LUMO: 2.37283 factor:1 | 1 (-1.21578) | -1 | -1 |
| G: -4176.47485 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10442.58743 HOMO: -6.49808 LUMO: 2.47351 factor:1 | 1 (-1.74689) | -1 | -1 |
| G: -4176.47485 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10442.61467 HOMO: -6.22052 LUMO: 1.86398 factor:1 | 1 (-1.77413) | -1 | -1 |
| G: -4176.47485 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10442.80327 HOMO: -6.32665 LUMO: 2.28031 factor:1 | 1 (-1.96273) | -1 | -1 |
| G: -4176.47485 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10442.45946 HOMO: -5.98378 LUMO: 2.16331 factor:1 | 1 (-1.61891) | -1 | -1 |
| G: -4176.47485 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10442.70912 HOMO: -6.08991 LUMO: 2.30208 factor:1 | 1 (-1.86858) | -1 | -1 |
| G: -4176.47485 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10441.91322 HOMO: -7.07224 LUMO: 1.55105 factor:1 | 1 (-1.07267) | 1 | 1 |
| G: -4176.47485 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10442.00663 HOMO: -6.84638 LUMO: 1.76874 factor:1 | 1 (-1.16609) | -1 | -1 |
| G: -4176.47485 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10440.86147 HOMO: -6.68856 LUMO: 1.47758 factor:1 | 1 (-0.02093) | -1 | -1 |
| G: -4176.47485 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10441.05595 HOMO: -6.69672 LUMO: 1.71976 factor:1 | 1 (-0.21541) | -1 | -1 |
| G: -4176.47485 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10441.88549 HOMO: -6.86543 LUMO: 2.24766 factor:1 | 1 (-1.04494) | -1 | -1 |
| G: -4176.47485 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10442.09918 HOMO: -7.21646 LUMO: 1.71976 factor:1 | 1 (-1.25864) | 1 | 1 |
| G: -4176.47485 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10441.88889 HOMO: -6.94162 LUMO: 2.21773 factor:1 | 1 (-1.04835) | -1 | -1 |
| G: -4176.47485 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10441.77036 HOMO: -6.34842 LUMO: 2.04358 factor:1 | 1 (-0.92981) | -1 | -1 |
| G: -4176.47485 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10441.62750 HOMO: -6.53345 LUMO: 1.96738 factor:1 | 1 (-0.78695) | -1 | -1 |
| G: -4176.47485 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10442.04802 HOMO: -6.34842 LUMO: 1.88303 factor:1 | 1 (-1.20748) | -1 | -1 |
| G: -4176.47485 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10441.52700 HOMO: -6.38651 LUMO: 2.08983 factor:1 | 1 (-0.68646) | -1 | -1 |
| G: -4176.47485 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10439.95285 HOMO: -6.01372 LUMO: 1.43676 factor:1 | -1 (0.88769) | -1 | -1 |
| G: -4176.47485 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10440.22935 HOMO: -6.30216 LUMO: 1.41771 factor:1 | -1 (0.61119) | -1 | -1 |
| G: -4176.47485 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10441.86576 HOMO: -6.52801 LUMO: 1.77146 factor:1 | 1 (-1.02522) | -1 | -1 |
| G: -4176.47485 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10442.01262 HOMO: -6.53617 LUMO: 1.72792 factor:1 | 1 (-1.17208) | -1 | -1 |
| G: -4176.47485 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10442.08976 HOMO: -6.56611 LUMO: 2.20412 factor:1 | 1 (-1.24922) | -1 | -1 |
| G: -4176.47485 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10442.47976 HOMO: -6.66679 LUMO: -0.72927 factor:1 | 1 (-1.63921) | -1 | -1 |
| G: -4176.47485 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10442.38944 HOMO: -6.85455 LUMO: -0.85444 factor:1 | 1 (-1.54890) | -1 | -1 |
| G: -4176.47485 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10443.26102 HOMO: -7.21646 LUMO: 0.27211 factor:1 | 1 (-2.42048) | 1 | 1 |
| G: -4176.47485 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10442.19306 HOMO: -6.57971 LUMO: -0.41361 factor:1 | 1 (-1.35251) | -1 | -1 |
| G: -4176.47485 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10442.10296 HOMO: -7.03142 LUMO: -1.14288 factor:1 | 1 (-1.26242) | -1 | -1 |
| G: -4176.47485 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10442.26343 HOMO: -6.29944 LUMO: 0.06803 factor:1 | 1 (-1.42288) | -1 | -1 |
| G: -4176.47485 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10442.20949 HOMO: -6.47359 LUMO: 0.28028 factor:1 | 1 (-1.36895) | -1 | -1 |
| G: -4176.47485 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10440.93848 HOMO: -6.42189 LUMO: 1.61364 factor:1 | 1 (-0.09793) | -1 | -1 |
| G: -4176.47485 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10440.87230 HOMO: -6.41100 LUMO: 1.80956 factor:1 | 1 (-0.03176) | -1 | -1 |
| G: -4176.47485 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10441.18596 HOMO: -6.83278 LUMO: 1.83949 factor:1 | 1 (-0.34542) | -1 | -1 |
| G: -4176.47485 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10442.45034 HOMO: -6.78380 LUMO: -0.76192 factor:1 | 1 (-1.60980) | -1 | -1 |
| G: -4176.47485 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10441.04063 HOMO: -6.95795 LUMO: 2.13609 factor:1 | 1 (-0.20009) | -1 | -1 |
| G: -4176.47485 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10440.81398 HOMO: -6.57155 LUMO: 1.89119 factor:1 | -1 (0.02656) | -1 | -1 |
| G: -4176.47485 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10442.05041 HOMO: -6.65591 LUMO: 1.93745 factor:1 | 1 (-1.20987) | -1 | -1 |
| G: -4176.47485 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10441.69490 HOMO: -6.44638 LUMO: 2.26943 factor:1 | 1 (-0.85436) | -1 | -1 |
| G: -4176.47485 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10441.54978 HOMO: -5.88038 LUMO: 1.90480 factor:1 | 1 (-0.70924) | -1 | -1 |
| G: -4176.47485 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10441.52845 HOMO: -6.22052 LUMO: 2.17691 factor:1 | 1 (-0.68790) | -1 | -1 |
| G: -4176.47485 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10442.31284 HOMO: -6.04637 LUMO: 2.23950 factor:1 | 1 (-1.47230) | -1 | -1 |
| G: -4176.47485 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10442.51453 HOMO: -6.44366 LUMO: 2.24766 factor:1 | 1 (-1.67399) | -1 | -1 |
| G: -4176.47485 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10442.80882 HOMO: -6.81917 LUMO: 2.08439 factor:1 | 1 (-1.96828) | -1 | -1 |
| G: -4176.47485 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10440.04643 HOMO: -6.48447 LUMO: 2.28576 factor:1 | -1 (0.79411) | -1 | -1 |
| G: -4176.47485 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10440.75858 HOMO: -6.54434 LUMO: 1.99187 factor:1 | -1 (0.08196) | -1 | -1 |
| G: -4614.53471 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10877.96349 HOMO: -6.17698 LUMO: -0.65852 factor:1 | -1 (0.93692) | -1 | -1 |
| G: -4614.53471 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10878.04175 HOMO: -6.08174 LUMO: -0.58504 factor:1 | -1 (0.85866) | -1 | -1 |
| G: -4614.53471 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10877.35300 HOMO: -6.55250 LUMO: -0.86804 factor:1 | -1 (1.54740) | -1 | -1 |
| G: -4614.53471 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10877.71845 HOMO: -6.57699 LUMO: -0.89525 factor:1 | -1 (1.18195) | -1 | -1 |
| G: -4614.53471 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10877.78966 HOMO: -6.63141 LUMO: -1.04220 factor:1 | -1 (1.11074) | -1 | -1 |
| G: -4614.53471 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10879.82047 HOMO: -6.69128 LUMO: -0.76736 factor:1 | 1 (-0.92007) | -1 | -1 |
| G: -4614.53471 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10879.13632 HOMO: -6.25318 LUMO: -1.03131 factor:1 | 1 (-0.23592) | -1 | -1 |
| G: -4614.53471 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10877.75094 HOMO: -6.69944 LUMO: 0.01905 factor:1 | -1 (1.14946) | -1 | -1 |
| G: -4614.53471 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10877.75782 HOMO: -6.28583 LUMO: 0.38368 factor:1 | -1 (1.14258) | -1 | -1 |
| G: -4614.53471 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10878.71395 HOMO: -6.90081 LUMO: -0.83811 factor:1 | -1 (0.18645) | -1 | -1 |
| G: -4614.53471 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10877.77793 HOMO: -6.78380 LUMO: -0.10068 factor:1 | -1 (1.12247) | -1 | -1 |
| G: -4614.53471 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10878.89501 HOMO: -6.30488 LUMO: -0.98505 factor:1 | -1 (0.00539) | -1 | -1 |
| G: -4614.53471 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10879.57451 HOMO: -6.29671 LUMO: -1.79051 factor:1 | 1 (-0.67411) | -1 | -1 |
| G: -4614.53471 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10878.93779 HOMO: -6.76747 LUMO: -0.22041 factor:1 | 1 (-0.03739) | -1 | -1 |
| G: -4614.53471 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10879.14824 HOMO: -6.22597 LUMO: -0.94968 factor:1 | 1 (-0.24784) | -1 | -1 |
| G: -4614.53471 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10877.76495 HOMO: -6.73482 LUMO: 0.05987 factor:1 | -1 (1.13545) | -1 | -1 |
| G: -4614.53471 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10877.73937 HOMO: -6.28855 LUMO: 0.34831 factor:1 | -1 (1.16103) | -1 | -1 |
| G: -4614.53471 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10876.39755 HOMO: -6.69400 LUMO: 0.25307 factor:1 | -1 (2.50285) | -1 | -1 |
| G: -4614.53471 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10877.02301 HOMO: -6.70216 LUMO: 0.61226 factor:1 | -1 (1.87740) | -1 | -1 |
| G: -4614.53471 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10878.67291 HOMO: -6.70216 LUMO: 0.17415 factor:1 | -1 (0.22749) | -1 | -1 |
| G: -4614.53471 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10878.02237 HOMO: -6.70761 LUMO: 0.24762 factor:1 | -1 (0.87803) | -1 | -1 |
| G: -4614.53471 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10878.73964 HOMO: -6.68856 LUMO: -0.84900 factor:1 | -1 (0.16076) | -1 | -1 |
| G: -4614.53471 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10877.76824 HOMO: -6.71033 LUMO: -0.38640 factor:1 | -1 (1.13216) | -1 | -1 |
| G: -4614.53471 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10877.61064 HOMO: -6.24501 LUMO: -0.09252 factor:1 | -1 (1.28977) | -1 | -1 |
| G: -4614.53471 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10877.54508 HOMO: -6.81645 LUMO: -0.07347 factor:1 | -1 (1.35532) | -1 | -1 |
| G: -4614.53471 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10877.75649 HOMO: -6.49536 LUMO: 0.09796 factor:1 | -1 (1.14391) | -1 | -1 |
| G: -4614.53471 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10877.57333 HOMO: -6.71033 LUMO: -0.26395 factor:1 | -1 (1.32707) | -1 | -1 |
| G: -4614.53471 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10877.65534 HOMO: -6.70489 LUMO: -0.09252 factor:1 | -1 (1.24506) | -1 | -1 |
| G: -4614.53471 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10877.72364 HOMO: -6.23685 LUMO: 0.39729 factor:1 | -1 (1.17676) | -1 | -1 |
| G: -4614.53471 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10878.64312 HOMO: -6.69400 LUMO: -0.05442 factor:1 | -1 (0.25728) | -1 | -1 |
| G: -4614.53471 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10878.32477 HOMO: -6.36202 LUMO: 0.09796 factor:1 | -1 (0.57563) | -1 | -1 |
| G: -4614.53471 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10877.68536 HOMO: -6.54978 LUMO: 0.15510 factor:1 | -1 (1.21504) | -1 | -1 |
| G: -4614.53471 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10877.80340 HOMO: -6.77836 LUMO: 0.25851 factor:1 | -1 (1.09700) | -1 | -1 |
| G: -4614.53471 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10881.00512 HOMO: -5.70623 LUMO: 0.73471 factor:1 | 1 (-2.10472) | -1 | -1 |
| G: -4614.53471 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10881.98351 HOMO: -5.58378 LUMO: 0.89253 factor:1 | 1 (-3.08310) | -1 | -1 |
| G: -4614.53471 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10881.46649 HOMO: -5.68718 LUMO: 0.87893 factor:1 | 1 (-2.56609) | -1 | -1 |
| G: -4614.53471 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10880.79543 HOMO: -5.10486 LUMO: 1.11567 factor:1 | 1 (-1.89503) | -1 | -1 |
| G: -4614.53471 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10880.73290 HOMO: -4.59328 LUMO: 1.27621 factor:1 | 1 (-1.83250) | -1 | -1 |
| G: -4614.53471 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10880.86776 HOMO: -4.45450 LUMO: 1.82044 factor:1 | 1 (-1.96736) | -1 | -1 |
| G: -4614.53471 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10880.81480 HOMO: -4.64226 LUMO: 1.70615 factor:1 | 1 (-1.91440) | -1 | -1 |
| G: -4614.53471 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10880.76873 HOMO: -5.04227 LUMO: 1.04492 factor:1 | 1 (-1.86833) | -1 | -1 |
| G: -4614.53471 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10880.67042 HOMO: -4.85723 LUMO: 0.93607 factor:1 | 1 (-1.77002) | -1 | -1 |
| G: -4614.53471 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10880.64881 HOMO: -4.72934 LUMO: 1.00410 factor:1 | 1 (-1.74841) | -1 | -1 |
| G: -4614.53471 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10880.77105 HOMO: -4.56335 LUMO: 1.56738 factor:1 | 1 (-1.87065) | -1 | -1 |
| G: -4614.53471 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10881.42850 HOMO: -5.48854 LUMO: 0.33198 factor:1 | 1 (-2.52810) | -1 | -1 |
| G: -4614.53471 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10880.47118 HOMO: -4.97424 LUMO: 1.33608 factor:1 | 1 (-1.57078) | -1 | -1 |
| G: -4614.53471 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10880.58228 HOMO: -4.60145 LUMO: 1.74697 factor:1 | 1 (-1.68188) | -1 | -1 |
| G: -4614.53471 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10881.73667 HOMO: -5.60010 LUMO: 0.74831 factor:1 | 1 (-2.83627) | -1 | -1 |
| G: -4614.53471 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10880.55926 HOMO: -5.66541 LUMO: 0.66668 factor:1 | 1 (-1.65886) | -1 | -1 |
| G: -4614.53471 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10880.96264 HOMO: -6.50080 LUMO: 0.07075 factor:1 | 1 (-2.06224) | -1 | -1 |
| G: -4614.53471 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10881.14338 HOMO: -5.79603 LUMO: 0.22313 factor:1 | 1 (-2.24298) | -1 | -1 |
| G: -4614.53471 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10880.27068 HOMO: -4.68036 LUMO: 1.29798 factor:1 | 1 (-1.37028) | -1 | -1 |
| G: -4614.53471 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10880.21030 HOMO: -4.84363 LUMO: 1.34424 factor:1 | 1 (-1.30990) | -1 | -1 |
| G: -4614.53471 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10880.38133 HOMO: -4.62321 LUMO: 1.82861 factor:1 | 1 (-1.48093) | -1 | -1 |
| G: -4614.53471 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10880.83015 HOMO: -5.83684 LUMO: 0.82178 factor:1 | 1 (-1.92975) | -1 | -1 |
| G: -4614.53471 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10880.32111 HOMO: -5.27629 LUMO: 0.57960 factor:1 | 1 (-1.42071) | -1 | -1 |
| G: -4614.53471 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10879.19632 HOMO: -5.15928 LUMO: -2.96876 factor:1 | 1 (-0.29592) | -1 | -1 |
| G: -4614.53471 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10880.60111 HOMO: -5.08853 LUMO: 0.89253 factor:1 | 1 (-1.70071) | -1 | -1 |
| G: -4614.53471 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10881.00300 HOMO: -6.42461 LUMO: 0.04354 factor:1 | 1 (-2.10260) | -1 | -1 |
| G: -4614.53471 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10880.96403 HOMO: -6.42733 LUMO: -0.00544 factor:1 | 1 (-2.06363) | -1 | -1 |
| G: -4614.53471 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10881.22594 HOMO: -5.87494 LUMO: 0.69933 factor:1 | 1 (-2.32554) | -1 | -1 |
| G: -4614.53471 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10880.33795 HOMO: -5.07492 LUMO: 1.02587 factor:1 | 1 (-1.43755) | -1 | -1 |
| G: -4614.53471 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10880.43401 HOMO: -4.44362 LUMO: 1.99187 factor:1 | 1 (-1.53361) | -1 | -1 |
| G: -4614.53471 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10880.77469 HOMO: -5.82052 LUMO: 0.43810 factor:1 | 1 (-1.87429) | -1 | -1 |
| G: -4614.53471 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10880.96877 HOMO: -5.75793 LUMO: 0.76464 factor:1 | 1 (-2.06836) | -1 | -1 |
| G: -4614.53471 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10880.52421 HOMO: -5.09669 LUMO: 0.72382 factor:1 | 1 (-1.62381) | -1 | -1 |
| G: -4614.53471 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10881.11748 HOMO: -6.75387 LUMO: -2.02453 factor:1 | 1 (-2.21707) | -1 | -1 |
| G: -4614.53471 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10880.71559 HOMO: -5.02322 LUMO: 1.14832 factor:1 | 1 (-1.81519) | -1 | -1 |
| G: -4614.53471 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10881.75090 HOMO: -5.75521 LUMO: 0.73471 factor:1 | 1 (-2.85050) | -1 | -1 |
| G: -4614.53471 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10880.69918 HOMO: -5.89943 LUMO: 0.54967 factor:1 | 1 (-1.79878) | -1 | -1 |
| G: -4614.53471 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10881.68271 HOMO: -5.80147 LUMO: 0.72382 factor:1 | 1 (-2.78231) | -1 | -1 |
| G: -4614.53471 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10880.93617 HOMO: -6.16066 LUMO: 0.39457 factor:1 | 1 (-2.03577) | -1 | -1 |
| G: -4614.53471 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10881.10575 HOMO: -5.98650 LUMO: 0.76736 factor:1 | 1 (-2.20535) | -1 | -1 |
| G: -4614.53471 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10880.39539 HOMO: -4.74839 LUMO: 1.88847 factor:1 | 1 (-1.49499) | -1 | -1 |
| G: -4614.53471 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10880.83540 HOMO: -5.62459 LUMO: 0.26939 factor:1 | 1 (-1.93500) | -1 | -1 |
| G: -4614.53471 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10880.22829 HOMO: -4.88172 LUMO: 1.30070 factor:1 | 1 (-1.32789) | -1 | -1 |
| G: -4614.53471 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10880.42832 HOMO: -5.09397 LUMO: 0.98505 factor:1 | 1 (-1.52792) | -1 | -1 |
| G: -4614.53471 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10880.93709 HOMO: -6.50080 LUMO: -0.28300 factor:1 | 1 (-2.03669) | -1 | -1 |
| G: -4614.53471 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10880.61434 HOMO: -5.04227 LUMO: 1.49935 factor:1 | 1 (-1.71394) | -1 | -1 |
| G: -4614.53471 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10880.62095 HOMO: -5.22731 LUMO: 0.88437 factor:1 | 1 (-1.72055) | -1 | -1 |
| G: -4614.53471 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10880.72030 HOMO: -4.95519 LUMO: 1.25717 factor:1 | 1 (-1.81990) | -1 | -1 |
| G: -4614.53471 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10880.81747 HOMO: -4.61233 LUMO: 1.27621 factor:1 | 1 (-1.91707) | -1 | -1 |
| G: -4614.53471 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10880.73548 HOMO: -4.70757 LUMO: 1.63813 factor:1 | 1 (-1.83508) | -1 | -1 |
| G: -4614.53471 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10880.55771 HOMO: -4.85179 LUMO: 1.11839 factor:1 | 1 (-1.65731) | -1 | -1 |
| G: -4614.53471 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10880.58133 HOMO: -4.97696 LUMO: 1.00138 factor:1 | 1 (-1.68093) | -1 | -1 |
| G: -4614.53471 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10881.66603 HOMO: -5.64636 LUMO: 0.81090 factor:1 | 1 (-2.76563) | -1 | -1 |
| G: -4614.53471 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10880.65597 HOMO: -4.37831 LUMO: 1.90208 factor:1 | 1 (-1.75557) | -1 | -1 |
| G: -4614.53471 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10880.52552 HOMO: -4.67764 LUMO: 1.54561 factor:1 | 1 (-1.62512) | -1 | -1 |
| G: -4614.53471 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10880.30154 HOMO: -5.87766 LUMO: 0.42994 factor:1 | 1 (-1.40114) | -1 | -1 |
| G: -4614.53471 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10880.60552 HOMO: -6.03821 LUMO: 0.32382 factor:1 | 1 (-1.70512) | -1 | -1 |
| G: -4614.53471 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10880.84278 HOMO: -5.99739 LUMO: 0.69389 factor:1 | 1 (-1.94238) | -1 | -1 |
| G: -4614.53471 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10880.36739 HOMO: -6.43821 LUMO: 0.15238 factor:1 | 1 (-1.46699) | -1 | -1 |
| G: -4614.53471 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10880.38002 HOMO: -6.63414 LUMO: -0.07347 factor:1 | 1 (-1.47962) | -1 | -1 |
| G: -4614.53471 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10880.68454 HOMO: -6.50080 LUMO: 0.10068 factor:1 | 1 (-1.78414) | -1 | -1 |
| G: -4614.53471 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10880.76098 HOMO: -6.49264 LUMO: 0.19592 factor:1 | 1 (-1.86058) | -1 | -1 |
| G: -4614.53471 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10880.63616 HOMO: -5.83956 LUMO: 0.12517 factor:1 | 1 (-1.73576) | -1 | -1 |
| G: -4614.53471 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10880.38696 HOMO: -6.50896 LUMO: 0.19048 factor:1 | 1 (-1.48656) | -1 | -1 |
| G: -4614.53471 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10880.66158 HOMO: -6.56611 LUMO: 0.04898 factor:1 | 1 (-1.76118) | -1 | -1 |
| G: -4614.53471 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10880.75799 HOMO: -6.68040 LUMO: -0.08436 factor:1 | 1 (-1.85759) | -1 | -1 |
| G: -4614.53471 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10880.87031 HOMO: -6.73754 LUMO: -0.08708 factor:1 | 1 (-1.96991) | -1 | -1 |
| G: -4614.53471 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10880.77976 HOMO: -6.80285 LUMO: -0.10612 factor:1 | 1 (-1.87935) | -1 | -1 |
| G: -4614.53471 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10880.83369 HOMO: -6.35658 LUMO: 0.02177 factor:1 | 1 (-1.93329) | -1 | -1 |
| G: -4614.53471 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10881.06958 HOMO: -5.74160 LUMO: 0.14694 factor:1 | 1 (-2.16918) | -1 | -1 |
| G: -4614.53471 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10880.18334 HOMO: -4.78376 LUMO: 0.92791 factor:1 | 1 (-1.28294) | -1 | -1 |
| G: -4614.53471 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10880.66947 HOMO: -5.90215 LUMO: 0.36463 factor:1 | 1 (-1.76907) | -1 | -1 |
| G: -4614.53471 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10880.12763 HOMO: -4.99329 LUMO: 0.85988 factor:1 | 1 (-1.22723) | -1 | -1 |
| G: -4614.53471 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10880.25390 HOMO: -4.93887 LUMO: 1.33608 factor:1 | 1 (-1.35349) | -1 | -1 |
| G: -4614.53471 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10880.37183 HOMO: -5.19193 LUMO: 0.50341 factor:1 | 1 (-1.47143) | -1 | -1 |
| G: -4614.53471 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10880.51918 HOMO: -6.64502 LUMO: -1.98643 factor:1 | 1 (-1.61878) | -1 | -1 |
| G: -4614.53471 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10880.62187 HOMO: -5.15384 LUMO: 0.94968 factor:1 | 1 (-1.72147) | -1 | -1 |
| G: -4614.53471 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10880.88093 HOMO: -6.31032 LUMO: 0.08436 factor:1 | 1 (-1.98053) | -1 | -1 |
| G: -4614.53471 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10880.19297 HOMO: -4.88716 LUMO: 0.82995 factor:1 | 1 (-1.29257) | -1 | -1 |
| G: -4614.53471 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10880.76520 HOMO: -5.57017 LUMO: 0.19320 factor:1 | 1 (-1.86480) | -1 | -1 |
| G: -4614.53471 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10880.10170 HOMO: -4.92254 LUMO: 0.93879 factor:1 | 1 (-1.20130) | -1 | -1 |
| G: -4614.53471 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10880.30337 HOMO: -4.77288 LUMO: 1.60003 factor:1 | 1 (-1.40296) | -1 | -1 |
| G: -4614.53471 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10880.48903 HOMO: -4.97696 LUMO: 0.89798 factor:1 | 1 (-1.58863) | -1 | -1 |
| G: -4614.53471 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10880.57719 HOMO: -5.00690 LUMO: 1.14288 factor:1 | 1 (-1.67679) | -1 | -1 |
| G: -4614.53471 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10880.75442 HOMO: -4.88444 LUMO: 1.48574 factor:1 | 1 (-1.85402) | -1 | -1 |
| G: -4614.53471 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10880.28454 HOMO: -5.03955 LUMO: 1.51023 factor:1 | 1 (-1.38413) | -1 | -1 |
| G: -4614.53471 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10880.02091 HOMO: -5.22459 LUMO: 0.99049 factor:1 | 1 (-1.12051) | -1 | -1 |
| G: -4614.53471 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10880.20168 HOMO: -5.29534 LUMO: 0.96056 factor:1 | 1 (-1.30128) | -1 | -1 |
| G: -4614.53471 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10880.37694 HOMO: -5.35520 LUMO: 0.68301 factor:1 | 1 (-1.47654) | -1 | -1 |
| G: -4614.53471 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10880.50517 HOMO: -5.27357 LUMO: 1.18642 factor:1 | 1 (-1.60476) | -1 | -1 |
| G: -4614.53471 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10881.50927 HOMO: -5.79875 LUMO: 0.61770 factor:1 | 1 (-2.60886) | -1 | -1 |
| G: -4614.53471 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10880.64797 HOMO: -7.64640 LUMO: -2.45175 factor:1 | 1 (-1.74757) | -1 | -1 |
| G: -4614.53471 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10880.68838 HOMO: -7.46953 LUMO: -1.29798 factor:1 | 1 (-1.78798) | 1 | 1 |
| G: -4614.53471 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10880.87072 HOMO: -7.95389 LUMO: -0.37280 factor:1 | 1 (-1.97032) | 1 | 1 |
| G: -4614.53471 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10880.47224 HOMO: -7.23279 LUMO: -1.19186 factor:1 | 1 (-1.57184) | 1 | 1 |
| G: -4614.53471 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10880.75499 HOMO: -7.14299 LUMO: -1.12927 factor:1 | 1 (-1.85459) | 1 | 1 |
| G: -4614.53471 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10879.90709 HOMO: -6.93074 LUMO: 0.31565 factor:1 | 1 (-1.00669) | -1 | -1 |
| G: -4614.53471 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10879.93906 HOMO: -6.63141 LUMO: 0.28028 factor:1 | 1 (-1.03866) | -1 | -1 |
| G: -4614.53471 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10879.90450 HOMO: -7.10489 LUMO: -1.07213 factor:1 | 1 (-1.00410) | 1 | 1 |
| G: -4614.53471 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10880.04962 HOMO: -7.00693 LUMO: -0.69389 factor:1 | 1 (-1.14922) | -1 | -1 |
| G: -4614.53471 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10881.21380 HOMO: -8.50356 LUMO: -1.79595 factor:1 | 1 (-2.31340) | -1 | -1 |
| G: -4614.53471 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10880.55246 HOMO: -7.79334 LUMO: -2.33746 factor:1 | 1 (-1.65206) | -1 | -1 |
| G: -4614.53471 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10880.76267 HOMO: -7.24367 LUMO: -0.85172 factor:1 | 1 (-1.86227) | 1 | 1 |
| G: -4614.53471 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10881.49215 HOMO: -7.94028 LUMO: -0.20136 factor:1 | 1 (-2.59175) | 1 | 1 |
| G: -4614.53471 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10880.35237 HOMO: -7.22462 LUMO: 0.84627 factor:1 | 1 (-1.45197) | 1 | 1 |
| G: -4614.53471 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10879.88513 HOMO: -6.54978 LUMO: 0.34831 factor:1 | 1 (-0.98473) | -1 | -1 |
| G: -4614.53471 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10879.97030 HOMO: -6.86815 LUMO: 0.32109 factor:1 | 1 (-1.06990) | -1 | -1 |
| G: -4614.53471 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10880.32924 HOMO: -7.17564 LUMO: -1.28438 factor:1 | 1 (-1.42884) | 1 | 1 |
| G: -4614.53471 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10880.93913 HOMO: -7.03142 LUMO: -1.12655 factor:1 | 1 (-2.03873) | -1 | -1 |
| G: -4614.53471 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10879.75979 HOMO: -7.39878 LUMO: 0.15783 factor:1 | 1 (-0.85939) | 1 | 1 |
| G: -4614.53471 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10879.77827 HOMO: -7.25728 LUMO: 0.42178 factor:1 | 1 (-0.87787) | 1 | 1 |
| G: -4614.53471 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10880.60704 HOMO: -6.86543 LUMO: 0.93879 factor:1 | 1 (-1.70664) | -1 | -1 |
| G: -4614.53471 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10880.30750 HOMO: -7.09673 LUMO: -0.69661 factor:1 | 1 (-1.40710) | 1 | 1 |
| G: -4614.53471 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10881.54440 HOMO: -7.74708 LUMO: 0.01088 factor:1 | 1 (-2.64399) | 1 | 1 |
| G: -4614.53471 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10879.32963 HOMO: -6.80557 LUMO: 0.46531 factor:1 | 1 (-0.42923) | -1 | -1 |
| G: -4614.53471 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10880.36116 HOMO: -7.29265 LUMO: 1.31975 factor:1 | 1 (-1.46076) | 1 | 1 |
| G: -4614.53471 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10879.65592 HOMO: -6.93618 LUMO: 0.29388 factor:1 | 1 (-0.75552) | -1 | -1 |
| G: -4614.53471 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10879.87729 HOMO: -6.53073 LUMO: 0.71022 factor:1 | 1 (-0.97689) | -1 | -1 |
| G: -4614.53471 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10880.43428 HOMO: -6.41917 LUMO: -1.24084 factor:1 | 1 (-1.53388) | -1 | -1 |
| G: -4614.53471 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10879.64686 HOMO: -6.67495 LUMO: -1.09118 factor:1 | 1 (-0.74646) | -1 | -1 |
| G: -4614.53471 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10879.62926 HOMO: -6.97156 LUMO: -0.53606 factor:1 | 1 (-0.72886) | -1 | -1 |
| G: -4614.53471 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10880.06214 HOMO: -6.85183 LUMO: -0.45715 factor:1 | 1 (-1.16174) | -1 | -1 |
| G: -4614.53471 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10879.81568 HOMO: -7.12666 LUMO: -0.67484 factor:1 | 1 (-0.91528) | 1 | 1 |
| G: -4614.53471 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10879.66194 HOMO: -7.49946 LUMO: -0.14694 factor:1 | 1 (-0.76154) | 1 | 1 |
| G: -4614.53471 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10879.82205 HOMO: -7.44231 LUMO: 0.58232 factor:1 | 1 (-0.92165) | 1 | 1 |
| G: -4614.53471 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10881.53569 HOMO: -7.36340 LUMO: -0.68301 factor:1 | 1 (-2.63529) | 1 | 1 |
| G: -4614.53471 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10881.01688 HOMO: -6.13073 LUMO: -0.54967 factor:1 | 1 (-2.11647) | -1 | -1 |
| G: -4614.53471 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10881.14768 HOMO: -7.81511 LUMO: -0.06531 factor:1 | 1 (-2.24728) | 1 | 1 |
| G: -4614.53471 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10880.51534 HOMO: -7.26816 LUMO: -1.02587 factor:1 | 1 (-1.61494) | 1 | 1 |
| G: -4614.53471 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10881.43868 HOMO: -7.98110 LUMO: -0.17960 factor:1 | 1 (-2.53828) | 1 | 1 |
| G: -4614.53471 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10880.26867 HOMO: -7.44776 LUMO: -1.00954 factor:1 | 1 (-1.36827) | 1 | 1 |
| G: -4614.53471 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10880.69706 HOMO: -7.47769 LUMO: -1.02859 factor:1 | 1 (-1.79666) | 1 | 1 |
| G: -4614.53471 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10880.20342 HOMO: -6.75659 LUMO: 0.39457 factor:1 | 1 (-1.30302) | -1 | -1 |
| G: -4614.53471 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10880.23670 HOMO: -6.71849 LUMO: 0.36735 factor:1 | 1 (-1.33630) | -1 | -1 |
| G: -4614.53471 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10880.83739 HOMO: -7.64096 LUMO: -1.43948 factor:1 | 1 (-1.93699) | 1 | 1 |
| G: -4614.53471 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10880.91263 HOMO: -7.83144 LUMO: -1.36601 factor:1 | 1 (-2.01223) | 1 | 1 |
| G: -4614.53471 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10880.08069 HOMO: -7.19469 LUMO: 0.35103 factor:1 | 1 (-1.18029) | 1 | 1 |
| G: -4614.53471 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10880.00608 HOMO: -7.03414 LUMO: 0.20409 factor:1 | 1 (-1.10568) | -1 | -1 |
| G: -4614.53471 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10879.62697 HOMO: -7.22734 LUMO: 0.31293 factor:1 | 1 (-0.72657) | 1 | 1 |
| G: -4614.53471 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10879.70390 HOMO: -6.93618 LUMO: 0.56055 factor:1 | 1 (-0.80350) | -1 | -1 |
| G: -4614.53471 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10880.47344 HOMO: -6.94707 LUMO: -0.88709 factor:1 | 1 (-1.57304) | -1 | -1 |
| G: -4614.53471 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10881.12763 HOMO: -6.86543 LUMO: -0.83267 factor:1 | 1 (-2.22722) | -1 | -1 |
| G: -4614.53471 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10880.83429 HOMO: -6.82189 LUMO: -1.15376 factor:1 | 1 (-1.93389) | -1 | -1 |
| G: -4614.53471 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10881.22330 HOMO: -6.65046 LUMO: -0.46531 factor:1 | 1 (-2.32290) | -1 | -1 |
| G: -4614.53471 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10879.60156 HOMO: -6.52529 LUMO: 0.20953 factor:1 | 1 (-0.70116) | -1 | -1 |
| G: -4614.53471 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10878.96130 HOMO: -6.80557 LUMO: 0.44355 factor:1 | 1 (-0.06090) | -1 | -1 |
| G: -4614.53471 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10880.95881 HOMO: -6.93074 LUMO: -0.81634 factor:1 | 1 (-2.05841) | -1 | -1 |
| G: -4614.53471 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10881.58323 HOMO: -7.43143 LUMO: -0.45987 factor:1 | 1 (-2.68282) | 1 | 1 |
| G: -4614.53471 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10882.45753 HOMO: -7.07224 LUMO: -0.68028 factor:1 | 1 (-3.55713) | 1 | 1 |
| G: -4614.53471 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10881.74339 HOMO: -6.68040 LUMO: -0.71566 factor:1 | 1 (-2.84299) | -1 | -1 |
| G: -4614.53471 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10880.83875 HOMO: -6.26406 LUMO: -1.09934 factor:1 | 1 (-1.93835) | -1 | -1 |
| G: -4614.53471 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10880.71088 HOMO: -5.94569 LUMO: -0.72110 factor:1 | 1 (-1.81048) | -1 | -1 |
| G: -4614.53471 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10881.43024 HOMO: -6.12256 LUMO: -0.42178 factor:1 | 1 (-2.52984) | -1 | -1 |
| G: -4614.53471 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10881.57321 HOMO: -6.09807 LUMO: 0.11429 factor:1 | 1 (-2.67281) | -1 | -1 |
| G: -4614.53471 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10881.62328 HOMO: -7.35252 LUMO: -0.55783 factor:1 | 1 (-2.72288) | 1 | 1 |
| G: -4614.53471 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10881.38956 HOMO: -7.57837 LUMO: -0.76736 factor:1 | 1 (-2.48916) | 1 | 1 |
| G: -4614.53471 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10881.49463 HOMO: -6.16066 LUMO: 0.01905 factor:1 | 1 (-2.59422) | -1 | -1 |
| G: -4614.53471 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10881.15124 HOMO: -6.13345 LUMO: -0.41906 factor:1 | 1 (-2.25084) | -1 | -1 |
| G: -4614.53471 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10881.18172 HOMO: -6.10351 LUMO: -0.33742 factor:1 | 1 (-2.28132) | -1 | -1 |
| G: -4614.53471 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10881.83746 HOMO: -7.24639 LUMO: -0.51702 factor:1 | 1 (-2.93706) | 1 | 1 |
| G: -4614.53471 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10880.96847 HOMO: -6.98244 LUMO: -1.82044 factor:1 | 1 (-2.06807) | -1 | -1 |
| G: -4614.53471 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10881.61659 HOMO: -6.37563 LUMO: -1.67622 factor:1 | 1 (-2.71619) | -1 | -1 |
| G: -4614.53471 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10880.20774 HOMO: -5.79058 LUMO: -2.55243 factor:1 | 1 (-1.30734) | -1 | -1 |
| G: -4614.53471 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10881.66298 HOMO: -6.34025 LUMO: -0.27483 factor:1 | 1 (-2.76258) | -1 | -1 |
| G: -4614.53471 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10881.14338 HOMO: -6.05453 LUMO: -0.51157 factor:1 | 1 (-2.24298) | -1 | -1 |
| G: -4614.53471 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10881.76249 HOMO: -7.53755 LUMO: -0.38912 factor:1 | 1 (-2.86209) | 1 | 1 |
| G: -4614.53471 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10882.52844 HOMO: -7.00421 LUMO: -0.50885 factor:1 | 1 (-3.62804) | -1 | -1 |
| G: -4614.53471 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10881.76149 HOMO: -7.52123 LUMO: -0.37552 factor:1 | 1 (-2.86109) | 1 | 1 |
| G: -4614.53471 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10881.87999 HOMO: -6.70489 LUMO: -1.04764 factor:1 | 1 (-2.97959) | -1 | -1 |
| G: -4614.53471 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10881.17059 HOMO: -7.06408 LUMO: -1.16737 factor:1 | 1 (-2.27019) | 1 | 1 |
| G: -4614.53471 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10881.73409 HOMO: -6.71849 LUMO: -1.02315 factor:1 | 1 (-2.83368) | -1 | -1 |
| G: -4614.53471 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10881.18036 HOMO: -6.16610 LUMO: -0.50885 factor:1 | 1 (-2.27996) | -1 | -1 |
| G: -4614.53471 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10879.80371 HOMO: -6.48447 LUMO: 0.07619 factor:1 | 1 (-0.90331) | -1 | -1 |
| G: -4614.53471 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10879.17809 HOMO: -7.06135 LUMO: 0.09796 factor:1 | 1 (-0.27769) | 1 | 1 |
| G: -4614.53471 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10879.74512 HOMO: -6.47359 LUMO: 0.22585 factor:1 | 1 (-0.84472) | -1 | -1 |
| G: -4614.53471 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10878.97129 HOMO: -6.10896 LUMO: -0.62314 factor:1 | 1 (-0.07089) | -1 | -1 |
| G: -4614.53471 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10877.74332 HOMO: -6.88176 LUMO: -0.96600 factor:1 | -1 (1.15708) | -1 | -1 |
| G: -4614.53471 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10879.73427 HOMO: -6.67495 LUMO: 0.21769 factor:1 | 1 (-0.83387) | -1 | -1 |
| G: -4614.53471 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10879.14168 HOMO: -6.84911 LUMO: 0.38368 factor:1 | 1 (-0.24128) | -1 | -1 |
| G: -4614.53471 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10881.00637 HOMO: -6.83550 LUMO: 1.29798 factor:1 | 1 (-2.10597) | -1 | -1 |
| G: -4614.53471 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10880.07950 HOMO: -6.67495 LUMO: 1.46941 factor:1 | 1 (-1.17910) | -1 | -1 |
| G: -4614.53471 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10880.94969 HOMO: -6.81917 LUMO: 1.30887 factor:1 | 1 (-2.04929) | -1 | -1 |
| G: -4614.53471 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10880.60264 HOMO: -6.56611 LUMO: 0.66396 factor:1 | 1 (-1.70224) | -1 | -1 |
| G: -4614.53471 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10879.84004 HOMO: -6.76203 LUMO: 0.60137 factor:1 | 1 (-0.93964) | -1 | -1 |
| G: -4614.53471 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10880.24211 HOMO: -6.55794 LUMO: 0.34286 factor:1 | 1 (-1.34171) | -1 | -1 |
| G: -4614.53471 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10880.22451 HOMO: -6.83550 LUMO: 0.35919 factor:1 | 1 (-1.32411) | -1 | -1 |
| G: -4614.53471 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10879.73236 HOMO: -7.17836 LUMO: 0.63130 factor:1 | 1 (-0.83196) | 1 | 1 |
| G: -4614.53471 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10879.33113 HOMO: -6.29944 LUMO: -0.69389 factor:1 | 1 (-0.43073) | -1 | -1 |
| G: -4614.53471 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10880.19887 HOMO: -7.06680 LUMO: -0.95784 factor:1 | 1 (-1.29847) | 1 | 1 |
| G: -4614.53471 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10880.00611 HOMO: -6.84638 LUMO: -0.87076 factor:1 | 1 (-1.10571) | -1 | -1 |
| G: -4614.53471 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10880.82161 HOMO: -6.96339 LUMO: -1.05308 factor:1 | 1 (-1.92121) | -1 | -1 |
| G: -4614.53471 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10879.68031 HOMO: -6.75387 LUMO: -1.04220 factor:1 | 1 (-0.77991) | -1 | -1 |
| G: -4614.53471 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10880.83992 HOMO: -6.71849 LUMO: -0.84355 factor:1 | 1 (-1.93952) | -1 | -1 |
| G: -4614.53471 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10879.25211 HOMO: -7.16748 LUMO: 0.51702 factor:1 | 1 (-0.35171) | 1 | 1 |
| G: -4614.53471 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10879.84197 HOMO: -6.92530 LUMO: 0.71566 factor:1 | 1 (-0.94157) | -1 | -1 |
| G: -4614.53471 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10878.29459 HOMO: -7.11034 LUMO: 0.01905 factor:1 | -1 (0.60581) | 1 | -1 |
| G: -4614.53471 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10879.18666 HOMO: -6.79468 LUMO: 0.77008 factor:1 | 1 (-0.28626) | -1 | -1 |
| G: -4614.53471 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10879.78521 HOMO: -6.52801 LUMO: 0.98233 factor:1 | 1 (-0.88481) | -1 | -1 |
| G: -4614.53471 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10878.96930 HOMO: -6.76475 LUMO: 0.53334 factor:1 | 1 (-0.06890) | -1 | -1 |
| G: -4614.53471 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10878.06229 HOMO: -5.29261 LUMO: 0.57416 factor:1 | -1 (0.83811) | -1 | -1 |
| G: -4614.53471 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10879.94453 HOMO: -6.57971 LUMO: 0.12789 factor:1 | 1 (-1.04413) | -1 | -1 |
| G: -4614.53471 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10879.13760 HOMO: -6.99333 LUMO: 0.51430 factor:1 | 1 (-0.23720) | -1 | -1 |
| G: -4614.53471 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10879.70387 HOMO: -6.41917 LUMO: 0.19048 factor:1 | 1 (-0.80347) | -1 | -1 |
| G: -4614.53471 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10877.09819 HOMO: -6.16066 LUMO: 1.77146 factor:1 | -1 (1.80221) | -1 | -1 |
| G: -4614.53471 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10877.02815 HOMO: -6.90353 LUMO: 1.65717 factor:1 | -1 (1.87225) | -1 | -1 |
| G: -4614.53471 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10877.29515 HOMO: -5.94569 LUMO: 1.29526 factor:1 | -1 (1.60525) | -1 | -1 |
| G: -4614.53471 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10879.83889 HOMO: -6.60420 LUMO: 1.33880 factor:1 | 1 (-0.93849) | -1 | -1 |
| G: -4614.53471 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10879.82934 HOMO: -6.23957 LUMO: 0.09524 factor:1 | 1 (-0.92894) | -1 | -1 |
| G: -4614.53471 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10880.75290 HOMO: -6.80013 LUMO: 1.34696 factor:1 | 1 (-1.85250) | -1 | -1 |
| G: -4614.53471 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10880.43934 HOMO: -7.53483 LUMO: -1.52384 factor:1 | 1 (-1.53894) | -1 | -1 |
| G: -4614.53471 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10880.41618 HOMO: -7.62463 LUMO: -1.65717 factor:1 | 1 (-1.51578) | -1 | -1 |
| G: -4614.53471 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10880.11419 HOMO: -7.62463 LUMO: -1.61364 factor:1 | 1 (-1.21379) | -1 | -1 |
| G: -4614.53471 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10880.57812 HOMO: -8.04096 LUMO: -1.66806 factor:1 | 1 (-1.67772) | -1 | -1 |
| G: -4614.53471 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10880.36837 HOMO: -7.18381 LUMO: -1.17553 factor:1 | 1 (-1.46797) | 1 | 1 |
| G: -4614.53471 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10880.77527 HOMO: -7.69538 LUMO: -1.36601 factor:1 | 1 (-1.87486) | 1 | 1 |
| G: -4614.53471 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10880.79600 HOMO: -7.95117 LUMO: -1.48302 factor:1 | 1 (-1.89560) | -1 | -1 |
| G: -4614.53471 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10879.77576 HOMO: -6.98516 LUMO: 0.35919 factor:1 | 1 (-0.87536) | -1 | -1 |
| G: -4614.53471 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10881.34755 HOMO: -7.91579 LUMO: -0.32109 factor:1 | 1 (-2.44715) | 1 | 1 |
| G: -4614.53471 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10879.55165 HOMO: -6.75659 LUMO: -0.03537 factor:1 | 1 (-0.65125) | -1 | -1 |
| G: -4614.53471 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10880.44394 HOMO: -7.78518 LUMO: -2.36467 factor:1 | 1 (-1.54354) | -1 | -1 |
| G: -4614.53471 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10880.58982 HOMO: -7.96477 LUMO: -2.75651 factor:1 | 1 (-1.68942) | -1 | -1 |
| G: -4614.53471 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10880.12380 HOMO: -7.60286 LUMO: -2.35106 factor:1 | 1 (-1.22340) | -1 | -1 |
| G: -4614.53471 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10880.13757 HOMO: -7.38245 LUMO: -1.21635 factor:1 | 1 (-1.23717) | 1 | 1 |
| G: -4614.53471 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10880.66865 HOMO: -7.91579 LUMO: -1.50479 factor:1 | 1 (-1.76825) | -1 | -1 |
| G: -4614.53471 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10881.03113 HOMO: -8.07362 LUMO: -0.28028 factor:1 | 1 (-2.13073) | 1 | 1 |
| G: -4614.53471 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10880.13670 HOMO: -7.38245 LUMO: -1.15921 factor:1 | 1 (-1.23629) | 1 | 1 |
| G: -4614.53471 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10880.41531 HOMO: -7.18653 LUMO: -0.94968 factor:1 | 1 (-1.51491) | 1 | 1 |
| G: -4614.53471 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10879.56071 HOMO: -6.88448 LUMO: 0.38096 factor:1 | 1 (-0.66031) | -1 | -1 |
| G: -4614.53471 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10878.60723 HOMO: -6.97972 LUMO: 0.43266 factor:1 | -1 (0.29318) | -1 | -1 |
| G: -4614.53471 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10879.71666 HOMO: -6.88992 LUMO: -0.43538 factor:1 | 1 (-0.81626) | -1 | -1 |
| G: -4614.53471 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10881.35119 HOMO: -7.97021 LUMO: -0.17143 factor:1 | 1 (-2.45079) | 1 | 1 |
| G: -4614.53471 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10880.11645 HOMO: -6.92530 LUMO: 0.77280 factor:1 | 1 (-1.21605) | -1 | -1 |
| G: -4614.53471 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10881.48673 HOMO: -7.89674 LUMO: -0.09796 factor:1 | 1 (-2.58633) | 1 | 1 |
| G: -4614.53471 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10880.09348 HOMO: -7.02870 LUMO: 0.88709 factor:1 | 1 (-1.19308) | -1 | -1 |
| G: -4614.53471 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10879.64137 HOMO: -6.78380 LUMO: 0.22041 factor:1 | 1 (-0.74097) | -1 | -1 |
| G: -4614.53471 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10880.69173 HOMO: -7.24911 LUMO: -0.82178 factor:1 | 1 (-1.79133) | 1 | 1 |
| G: -4614.53471 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10879.45889 HOMO: -6.77019 LUMO: 0.52790 factor:1 | 1 (-0.55849) | -1 | -1 |
| G: -4614.53471 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10881.08436 HOMO: -8.56070 LUMO: -1.83405 factor:1 | 1 (-2.18396) | -1 | -1 |
| G: -4614.53471 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10880.19580 HOMO: -7.74164 LUMO: -2.36195 factor:1 | 1 (-1.29540) | -1 | -1 |
| G: -4614.53471 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10880.21607 HOMO: -7.39878 LUMO: -2.41637 factor:1 | 1 (-1.31567) | -1 | -1 |
| G: -4614.53471 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10880.43093 HOMO: -7.61647 LUMO: -2.34018 factor:1 | 1 (-1.53053) | -1 | -1 |
| G: -4614.53471 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10879.64262 HOMO: -6.93346 LUMO: -0.57688 factor:1 | 1 (-0.74222) | -1 | -1 |
| G: -4614.53471 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10880.87211 HOMO: -6.85183 LUMO: -1.00410 factor:1 | 1 (-1.97171) | -1 | -1 |
| G: -4614.53471 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10880.18350 HOMO: -7.18925 LUMO: -1.12655 factor:1 | 1 (-1.28310) | 1 | 1 |
| G: -4614.53471 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10880.09588 HOMO: -6.85183 LUMO: -1.60275 factor:1 | 1 (-1.19548) | -1 | -1 |
| G: -4614.53471 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10879.69424 HOMO: -7.51578 LUMO: 0.12517 factor:1 | 1 (-0.79384) | 1 | 1 |
| G: -4614.53471 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10879.65331 HOMO: -7.36068 LUMO: 0.05714 factor:1 | 1 (-0.75291) | 1 | 1 |
| G: -4614.53471 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10879.84559 HOMO: -7.49674 LUMO: 0.18776 factor:1 | 1 (-0.94519) | 1 | 1 |
| G: -4614.53471 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10880.11781 HOMO: -7.09401 LUMO: -1.24900 factor:1 | 1 (-1.21741) | 1 | 1 |
| G: -4614.53471 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10879.84221 HOMO: -7.22462 LUMO: -1.61364 factor:1 | 1 (-0.94181) | -1 | -1 |
| G: -4614.53471 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10879.65563 HOMO: -7.74436 LUMO: -0.18776 factor:1 | 1 (-0.75522) | 1 | 1 |
| G: -4614.53471 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10879.75032 HOMO: -7.35252 LUMO: 0.75376 factor:1 | 1 (-0.84992) | 1 | 1 |
| G: -4614.53471 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10879.58852 HOMO: -7.75252 LUMO: 0.00816 factor:1 | 1 (-0.68812) | 1 | 1 |
| G: -4614.53471 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10879.28895 HOMO: -7.06680 LUMO: 0.24490 factor:1 | 1 (-0.38855) | 1 | 1 |
| G: -4614.53471 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10879.61043 HOMO: -7.49129 LUMO: 0.14150 factor:1 | 1 (-0.71003) | 1 | 1 |
| G: -4614.53471 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10880.65181 HOMO: -6.90625 LUMO: -1.11295 factor:1 | 1 (-1.75141) | -1 | -1 |
| G: -4614.53471 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10880.63417 HOMO: -6.78380 LUMO: -0.93063 factor:1 | 1 (-1.73377) | -1 | -1 |
| G: -4614.53471 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10880.23623 HOMO: -7.79878 LUMO: 0.30477 factor:1 | 1 (-1.33583) | 1 | 1 |
| G: -4614.53471 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10880.35417 HOMO: -7.87498 LUMO: 0.61770 factor:1 | 1 (-1.45377) | 1 | 1 |
| G: -4614.53471 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10880.21199 HOMO: -7.23823 LUMO: 0.30205 factor:1 | 1 (-1.31159) | 1 | 1 |
| G: -4614.53471 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10879.54003 HOMO: -7.67633 LUMO: 0.13061 factor:1 | 1 (-0.63963) | 1 | 1 |
| G: -4614.53471 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10879.56477 HOMO: -7.79606 LUMO: 0.34558 factor:1 | 1 (-0.66437) | 1 | 1 |
| G: -4614.53471 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10879.61682 HOMO: -6.66135 LUMO: -2.60141 factor:1 | 1 (-0.71642) | -1 | -1 |
| G: -4614.53471 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10879.68300 HOMO: -7.03142 LUMO: 0.50885 factor:1 | 1 (-0.78260) | -1 | -1 |
| G: -4614.53471 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10879.65065 HOMO: -7.05591 LUMO: -0.06531 factor:1 | 1 (-0.75025) | -1 | -1 |
| G: -4614.53471 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10880.23719 HOMO: -7.45592 LUMO: -1.39594 factor:1 | 1 (-1.33679) | 1 | 1 |
| G: -4614.53471 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10880.40092 HOMO: -7.22462 LUMO: -1.10478 factor:1 | 1 (-1.50052) | 1 | 1 |
| G: -4614.53471 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10880.93483 HOMO: -8.14709 LUMO: -0.55783 factor:1 | 1 (-2.03443) | 1 | 1 |
| G: -4614.53471 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10880.13776 HOMO: -7.22190 LUMO: -1.14560 factor:1 | 1 (-1.23736) | 1 | 1 |
| G: -4614.53471 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10880.42388 HOMO: -7.28721 LUMO: -1.14016 factor:1 | 1 (-1.52348) | 1 | 1 |
| G: -4614.53471 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10879.52414 HOMO: -6.97156 LUMO: 0.51702 factor:1 | 1 (-0.62374) | -1 | -1 |
| G: -4614.53471 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10878.59577 HOMO: -7.37156 LUMO: 0.29388 factor:1 | -1 (0.30463) | 1 | -1 |
| G: -4614.53471 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10880.14244 HOMO: -7.66273 LUMO: -1.59731 factor:1 | 1 (-1.24204) | -1 | -1 |
| G: -4614.53471 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10880.12793 HOMO: -7.50490 LUMO: -1.49935 factor:1 | 1 (-1.22753) | -1 | -1 |
| G: -4614.53471 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10880.33991 HOMO: -7.61102 LUMO: -1.45581 factor:1 | 1 (-1.43951) | 1 | 1 |
| G: -4614.53471 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10880.44503 HOMO: -7.58653 LUMO: -1.61091 factor:1 | 1 (-1.54463) | -1 | -1 |
| G: -4614.53471 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10880.76340 HOMO: -7.36068 LUMO: -1.14560 factor:1 | 1 (-1.86300) | 1 | 1 |
| G: -4614.53471 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10879.62202 HOMO: -6.96339 LUMO: 0.26939 factor:1 | 1 (-0.72162) | -1 | -1 |
| G: -4614.53471 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10879.45219 HOMO: -6.53617 LUMO: 0.22313 factor:1 | 1 (-0.55179) | -1 | -1 |
| G: -4614.53471 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10880.30048 HOMO: -7.33619 LUMO: -1.02587 factor:1 | 1 (-1.40008) | 1 | 1 |
| G: -4614.53471 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10879.98243 HOMO: -6.87904 LUMO: 0.33742 factor:1 | 1 (-1.08203) | -1 | -1 |
| G: -4614.53471 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10879.84951 HOMO: -6.88448 LUMO: 0.58777 factor:1 | 1 (-0.94911) | -1 | -1 |
| G: -4614.53471 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10879.69160 HOMO: -6.55522 LUMO: -1.51295 factor:1 | 1 (-0.79120) | -1 | -1 |
| G: -4614.53471 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10879.15910 HOMO: -7.43415 LUMO: 0.10612 factor:1 | 1 (-0.25870) | 1 | 1 |
| G: -4614.53471 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10879.52553 HOMO: -7.54300 LUMO: -0.02449 factor:1 | 1 (-0.62513) | 1 | 1 |
| G: -4614.53471 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10879.44104 HOMO: -7.42054 LUMO: 0.28028 factor:1 | 1 (-0.54064) | 1 | 1 |
| G: -4614.53471 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10879.63720 HOMO: -6.98244 LUMO: -0.95784 factor:1 | 1 (-0.73680) | -1 | -1 |
| G: -4614.53471 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10879.68602 HOMO: -6.96884 LUMO: -1.12383 factor:1 | 1 (-0.78562) | -1 | -1 |
| G: -4614.53471 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10880.60628 HOMO: -6.80829 LUMO: -0.98233 factor:1 | 1 (-1.70588) | -1 | -1 |
| G: -4614.53471 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10879.62036 HOMO: -7.60830 LUMO: 0.58504 factor:1 | 1 (-0.71996) | 1 | 1 |
| G: -4614.53471 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10879.12435 HOMO: -7.52123 LUMO: 0.08163 factor:1 | 1 (-0.22395) | 1 | 1 |
| G: -4614.53471 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10879.42419 HOMO: -7.59742 LUMO: 0.00272 factor:1 | 1 (-0.52379) | 1 | 1 |
| G: -4614.53471 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10879.91419 HOMO: -6.99333 LUMO: -1.33880 factor:1 | 1 (-1.01379) | -1 | -1 |
| G: -4614.53471 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10879.50887 HOMO: -6.63958 LUMO: -1.39322 factor:1 | 1 (-0.60847) | -1 | -1 |
| G: -4614.53471 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10879.58640 HOMO: -7.86137 LUMO: 0.01633 factor:1 | 1 (-0.68600) | 1 | 1 |
| G: -4614.53471 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10879.32093 HOMO: -7.29537 LUMO: 0.14694 factor:1 | 1 (-0.42052) | 1 | 1 |
| G: -4614.53471 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10879.63016 HOMO: -6.95523 LUMO: 0.48708 factor:1 | 1 (-0.72975) | -1 | -1 |
| G: -4614.53471 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10880.11487 HOMO: -7.10217 LUMO: -1.10478 factor:1 | 1 (-1.21447) | 1 | 1 |
| G: -4614.53471 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10881.12855 HOMO: -6.88176 LUMO: -0.96328 factor:1 | 1 (-2.22815) | -1 | -1 |
| G: -4614.53471 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10879.62605 HOMO: -7.89130 LUMO: -0.13334 factor:1 | 1 (-0.72565) | 1 | 1 |
| G: -4614.53471 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10879.50180 HOMO: -7.75252 LUMO: 0.25579 factor:1 | 1 (-0.60140) | 1 | 1 |
| G: -4614.53471 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10880.89540 HOMO: -6.87632 LUMO: -0.93063 factor:1 | 1 (-1.99500) | -1 | -1 |
| G: -4614.53471 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10881.70641 HOMO: -6.78108 LUMO: -0.86804 factor:1 | 1 (-2.80601) | -1 | -1 |
| G: -4614.53471 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10881.49814 HOMO: -5.98106 LUMO: 0.10340 factor:1 | 1 (-2.59773) | -1 | -1 |
| G: -4614.53471 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10880.90610 HOMO: -6.40284 LUMO: -0.87349 factor:1 | 1 (-2.00570) | -1 | -1 |
| G: -4614.53471 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10881.03279 HOMO: -6.77019 LUMO: -1.20819 factor:1 | 1 (-2.13239) | -1 | -1 |
| G: -4614.53471 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10880.25572 HOMO: -6.90081 LUMO: -1.00682 factor:1 | 1 (-1.35532) | -1 | -1 |
| G: -4614.53471 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10878.50559 HOMO: -6.59060 LUMO: -0.26667 factor:1 | -1 (0.39481) | -1 | -1 |
| G: -4614.53471 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10879.34498 HOMO: -6.50896 LUMO: -0.48708 factor:1 | 1 (-0.44458) | -1 | -1 |
| G: -4614.53471 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10879.04465 HOMO: -6.20420 LUMO: -0.73471 factor:1 | 1 (-0.14425) | -1 | -1 |
| G: -4614.53471 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10879.05951 HOMO: -6.17154 LUMO: -0.68573 factor:1 | 1 (-0.15910) | -1 | -1 |
| G: -4614.53471 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10879.44441 HOMO: -6.21236 LUMO: 0.09796 factor:1 | 1 (-0.54401) | -1 | -1 |
| G: -4614.53471 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10879.25366 HOMO: -6.38379 LUMO: 0.58232 factor:1 | 1 (-0.35326) | -1 | -1 |
| G: -4614.53471 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10880.55828 HOMO: -7.42871 LUMO: 0.40273 factor:1 | 1 (-1.65788) | 1 | 1 |
| G: -4614.53471 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10880.65850 HOMO: -6.54978 LUMO: 0.26395 factor:1 | 1 (-1.75810) | -1 | -1 |
| G: -4614.53471 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10879.97607 HOMO: -7.14027 LUMO: 0.14150 factor:1 | 1 (-1.07567) | 1 | 1 |
| G: -4614.53471 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10880.52214 HOMO: -7.25456 LUMO: -0.15783 factor:1 | 1 (-1.62174) | 1 | 1 |
| G: -4614.53471 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10879.91685 HOMO: -6.90897 LUMO: 0.63403 factor:1 | 1 (-1.01645) | -1 | -1 |
| G: -4614.53471 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10880.63104 HOMO: -6.49264 LUMO: 0.71022 factor:1 | 1 (-1.73064) | -1 | -1 |
| G: -4614.53471 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10879.69497 HOMO: -6.56067 LUMO: -1.03947 factor:1 | 1 (-0.79457) | -1 | -1 |
| G: -4614.53471 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10880.34927 HOMO: -6.79196 LUMO: -1.12655 factor:1 | 1 (-1.44887) | -1 | -1 |
| G: -4614.53471 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10879.90341 HOMO: -6.95251 LUMO: -1.09118 factor:1 | 1 (-1.00301) | -1 | -1 |
| G: -4614.53471 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10879.55266 HOMO: -7.47225 LUMO: -0.22041 factor:1 | 1 (-0.65226) | 1 | 1 |
| G: -4614.53471 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10880.71872 HOMO: -7.13483 LUMO: -0.98505 factor:1 | 1 (-1.81832) | 1 | 1 |
| G: -4614.53471 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10880.73913 HOMO: -6.99061 LUMO: -1.05852 factor:1 | 1 (-1.83873) | -1 | -1 |
| G: -4614.53471 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10880.64528 HOMO: -6.52257 LUMO: -1.11022 factor:1 | 1 (-1.74488) | -1 | -1 |
| G: -4614.53471 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10881.51501 HOMO: -6.75114 LUMO: -1.09934 factor:1 | 1 (-2.61461) | -1 | -1 |
| G: -4614.53471 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10881.45416 HOMO: -6.82189 LUMO: -0.89253 factor:1 | 1 (-2.55376) | -1 | -1 |
| G: -4614.53471 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10881.39226 HOMO: -6.83278 LUMO: -0.97961 factor:1 | 1 (-2.49186) | -1 | -1 |
| G: -4614.53471 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10880.87938 HOMO: -6.65318 LUMO: -0.84355 factor:1 | 1 (-1.97898) | -1 | -1 |
| G: -4614.53471 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10880.79053 HOMO: -6.75931 LUMO: -0.88437 factor:1 | 1 (-1.89013) | -1 | -1 |
| G: -4614.53471 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10880.75673 HOMO: -6.19059 LUMO: -0.45715 factor:1 | 1 (-1.85633) | -1 | -1 |
| G: -4614.53471 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10880.61287 HOMO: -7.09673 LUMO: -2.01908 factor:1 | 1 (-1.71247) | -1 | -1 |
| G: -4614.53471 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10880.24472 HOMO: -7.88042 LUMO: 0.38640 factor:1 | 1 (-1.34432) | 1 | 1 |
| G: -4614.53471 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10880.36715 HOMO: -7.83144 LUMO: 0.14422 factor:1 | 1 (-1.46675) | 1 | 1 |
| G: -4614.53471 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10880.20872 HOMO: -7.46408 LUMO: 0.44627 factor:1 | 1 (-1.30832) | 1 | 1 |
| G: -4614.53471 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10880.54922 HOMO: -7.12394 LUMO: -2.04902 factor:1 | 1 (-1.64882) | -1 | -1 |
| G: -4614.53471 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10880.86348 HOMO: -6.78380 LUMO: -1.11295 factor:1 | 1 (-1.96308) | -1 | -1 |
| G: -4614.53471 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10881.58886 HOMO: -7.12938 LUMO: -0.23674 factor:1 | 1 (-2.68846) | 1 | 1 |
| G: -4614.53471 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10881.38711 HOMO: -6.14705 LUMO: -0.20409 factor:1 | 1 (-2.48671) | -1 | -1 |
| G: -4614.53471 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10880.93704 HOMO: -6.50080 LUMO: -0.28300 factor:1 | 1 (-2.03664) | -1 | -1 |
| G: -4614.53471 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10880.39945 HOMO: -6.50352 LUMO: -0.62042 factor:1 | 1 (-1.49905) | -1 | -1 |
| G: -4614.53471 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10881.12316 HOMO: -6.46543 LUMO: -0.53879 factor:1 | 1 (-2.22276) | -1 | -1 |
| G: -4614.53471 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10881.72775 HOMO: -7.32803 LUMO: -0.52790 factor:1 | 1 (-2.82734) | 1 | 1 |
| G: -4614.53471 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10881.14123 HOMO: -5.94025 LUMO: -0.17687 factor:1 | 1 (-2.24083) | -1 | -1 |
| G: -4614.53471 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10881.04798 HOMO: -5.62187 LUMO: 0.05714 factor:1 | 1 (-2.14758) | -1 | -1 |
| G: -4614.53471 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10880.34753 HOMO: -7.03414 LUMO: -1.04492 factor:1 | 1 (-1.44713) | -1 | -1 |
| G: -4614.53471 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10881.11712 HOMO: -6.75387 LUMO: -2.02181 factor:1 | 1 (-2.21672) | -1 | -1 |
| G: -4614.53471 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10881.04607 HOMO: -6.55250 LUMO: -0.75648 factor:1 | 1 (-2.14567) | -1 | -1 |
| G: -4614.53471 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10880.44318 HOMO: -6.81101 LUMO: -1.02043 factor:1 | 1 (-1.54278) | -1 | -1 |
| G: -4614.53471 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10879.57802 HOMO: -6.69672 LUMO: -2.81910 factor:1 | 1 (-0.67762) | -1 | -1 |
| G: -4614.53471 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10879.29361 HOMO: -6.69128 LUMO: -2.58236 factor:1 | 1 (-0.39320) | -1 | -1 |
| G: -4614.53471 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10880.52443 HOMO: -6.73482 LUMO: -2.06807 factor:1 | 1 (-1.62403) | -1 | -1 |
| G: -4614.53471 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10879.43682 HOMO: -7.66545 LUMO: 0.17143 factor:1 | 1 (-0.53642) | 1 | 1 |
| G: -4614.53471 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10878.00438 HOMO: -6.87904 LUMO: -1.25172 factor:1 | -1 (0.89602) | -1 | -1 |
| G: -4614.53471 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10878.05693 HOMO: -6.84366 LUMO: -0.19320 factor:1 | -1 (0.84347) | -1 | -1 |
| G: -4614.53471 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10878.90285 HOMO: -6.97972 LUMO: -0.97961 factor:1 | 1 (-0.00245) | -1 | -1 |
| G: -4614.53471 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10879.05355 HOMO: -6.72121 LUMO: -0.70477 factor:1 | 1 (-0.15315) | -1 | -1 |
| G: -4614.53471 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10878.97118 HOMO: -7.18925 LUMO: 0.40001 factor:1 | 1 (-0.07078) | 1 | 1 |
| G: -4614.53471 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10879.51456 HOMO: -6.72121 LUMO: 0.19592 factor:1 | 1 (-0.61416) | -1 | -1 |
| G: -4614.53471 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10879.20694 HOMO: -6.85999 LUMO: -0.39457 factor:1 | 1 (-0.30654) | -1 | -1 |
| G: -4614.53471 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10879.85538 HOMO: -6.90625 LUMO: 0.05987 factor:1 | 1 (-0.95498) | -1 | -1 |
| G: -4614.53471 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10879.19646 HOMO: -7.00421 LUMO: 0.37552 factor:1 | 1 (-0.29606) | -1 | -1 |
| G: -4614.53471 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10879.03499 HOMO: -6.56883 LUMO: -0.97689 factor:1 | 1 (-0.13459) | -1 | -1 |
| G: -4614.53471 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10879.76760 HOMO: -6.66679 LUMO: 0.56055 factor:1 | 1 (-0.86720) | -1 | -1 |
| G: -4614.53471 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10879.71478 HOMO: -6.75931 LUMO: 0.32926 factor:1 | 1 (-0.81438) | -1 | -1 |
| G: -4614.53471 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10879.01586 HOMO: -6.53617 LUMO: -1.06397 factor:1 | 1 (-0.11546) | -1 | -1 |
| G: -4614.53471 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10879.39331 HOMO: -6.78108 LUMO: 0.42722 factor:1 | 1 (-0.49291) | -1 | -1 |
| G: -4614.53471 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10879.83117 HOMO: -7.05319 LUMO: 0.61498 factor:1 | 1 (-0.93077) | -1 | -1 |
| G: -4614.53471 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10880.03914 HOMO: -6.78380 LUMO: 1.49391 factor:1 | 1 (-1.13874) | -1 | -1 |
| G: -4614.53471 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10880.36456 HOMO: -7.21102 LUMO: 0.27211 factor:1 | 1 (-1.46416) | 1 | 1 |
| G: -4614.53471 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10880.58775 HOMO: -6.67223 LUMO: 0.81362 factor:1 | 1 (-1.68735) | -1 | -1 |
| G: -4614.53471 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10880.85546 HOMO: -6.69944 LUMO: 1.40683 factor:1 | 1 (-1.95506) | -1 | -1 |
| G: -4614.53471 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10880.92721 HOMO: -7.02598 LUMO: 1.46941 factor:1 | 1 (-2.02681) | -1 | -1 |
| G: -4614.53471 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10878.70742 HOMO: -5.85045 LUMO: -0.76736 factor:1 | -1 (0.19298) | -1 | -1 |
| G: -4614.53471 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10879.21453 HOMO: -6.53890 LUMO: -0.50885 factor:1 | 1 (-0.31413) | -1 | -1 |
| G: -4614.53471 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10878.93847 HOMO: -6.42733 LUMO: -0.63947 factor:1 | 1 (-0.03807) | -1 | -1 |
| G: -4614.53471 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10878.75656 HOMO: -6.82189 LUMO: -0.85444 factor:1 | -1 (0.14384) | -1 | -1 |
| G: -4614.53471 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10878.73966 HOMO: -6.97428 LUMO: -1.22179 factor:1 | -1 (0.16074) | -1 | -1 |
| G: -4614.53471 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10880.84928 HOMO: -6.93346 LUMO: -1.09934 factor:1 | 1 (-1.94888) | -1 | -1 |
| G: -4614.53471 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10880.13136 HOMO: -7.17292 LUMO: -1.11839 factor:1 | 1 (-1.23096) | 1 | 1 |
| G: -4614.53471 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10880.70332 HOMO: -7.00965 LUMO: -1.23268 factor:1 | 1 (-1.80292) | -1 | -1 |
| G: -4614.53471 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10880.77586 HOMO: -6.73210 LUMO: -1.12383 factor:1 | 1 (-1.87546) | -1 | -1 |
| G: -4614.53471 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10879.68131 HOMO: -7.61375 LUMO: -0.11973 factor:1 | 1 (-0.78091) | 1 | 1 |
| G: -4614.53471 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10879.85277 HOMO: -7.42327 LUMO: 0.41906 factor:1 | 1 (-0.95237) | 1 | 1 |
| G: -4614.53471 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10881.21876 HOMO: -6.94162 LUMO: -1.01771 factor:1 | 1 (-2.31836) | -1 | -1 |
| G: -4614.53471 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10880.80430 HOMO: -6.82189 LUMO: -0.92791 factor:1 | 1 (-1.90390) | -1 | -1 |
| G: -4614.53471 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10880.68397 HOMO: -6.92258 LUMO: -1.73881 factor:1 | 1 (-1.78357) | -1 | -1 |
| G: -4614.53471 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10881.46790 HOMO: -6.50896 LUMO: -1.60819 factor:1 | 1 (-2.56750) | -1 | -1 |
| G: -4614.53471 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10880.52130 HOMO: -6.38379 LUMO: -2.18780 factor:1 | 1 (-1.62090) | -1 | -1 |
| G: -4614.53471 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10880.67412 HOMO: -6.48992 LUMO: -0.97417 factor:1 | 1 (-1.77372) | -1 | -1 |
| G: -4614.53471 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10881.22556 HOMO: -6.01644 LUMO: -0.04354 factor:1 | 1 (-2.32516) | -1 | -1 |
| G: -4614.53471 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10880.76022 HOMO: -6.70761 LUMO: -0.14422 factor:1 | 1 (-1.85982) | -1 | -1 |
| G: -4614.53471 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10881.03802 HOMO: -6.70216 LUMO: 0.14422 factor:1 | 1 (-2.13762) | -1 | -1 |
| G: -4614.53471 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10880.21749 HOMO: -7.07224 LUMO: -0.10885 factor:1 | 1 (-1.31709) | 1 | 1 |
| G: -4614.53471 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10881.27451 HOMO: -7.52667 LUMO: -0.74287 factor:1 | 1 (-2.37411) | 1 | 1 |
| G: -4614.53471 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10880.74849 HOMO: -6.48447 LUMO: -0.96056 factor:1 | 1 (-1.84809) | -1 | -1 |
| G: -4614.53471 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10881.26428 HOMO: -6.22597 LUMO: -0.41361 factor:1 | 1 (-2.36388) | -1 | -1 |
| G: -4614.53471 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10880.90626 HOMO: -6.12256 LUMO: -1.05852 factor:1 | 1 (-2.00586) | -1 | -1 |
| G: -4614.53471 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10879.69824 HOMO: -6.97428 LUMO: -0.60681 factor:1 | 1 (-0.79784) | -1 | -1 |
| G: -4614.53471 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10880.28296 HOMO: -6.78380 LUMO: -0.88981 factor:1 | 1 (-1.38256) | -1 | -1 |
| G: -4614.53471 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10880.89573 HOMO: -6.85999 LUMO: 0.07891 factor:1 | 1 (-1.99533) | -1 | -1 |
| G: -4614.53471 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10880.98915 HOMO: -7.08312 LUMO: -0.60137 factor:1 | 1 (-2.08875) | 1 | 1 |
| G: -4614.53471 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10880.46448 HOMO: -6.57699 LUMO: -0.68028 factor:1 | 1 (-1.56408) | -1 | -1 |
| G: -4614.53471 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10880.69529 HOMO: -6.09807 LUMO: -0.31837 factor:1 | 1 (-1.79489) | -1 | -1 |
| G: -4614.53471 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10881.22833 HOMO: -6.10624 LUMO: 0.14966 factor:1 | 1 (-2.32793) | -1 | -1 |
| G: -4614.53471 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10880.07220 HOMO: -6.77019 LUMO: -0.95784 factor:1 | 1 (-1.17180) | -1 | -1 |
| G: -4614.53471 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10880.95932 HOMO: -5.93208 LUMO: -0.44627 factor:1 | 1 (-2.05892) | -1 | -1 |
| G: -4614.53471 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10881.71175 HOMO: -6.12256 LUMO: -0.27756 factor:1 | 1 (-2.81134) | -1 | -1 |
| G: -4614.53471 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10881.11086 HOMO: -5.98106 LUMO: -0.37824 factor:1 | 1 (-2.21046) | -1 | -1 |
| G: -4614.53471 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10881.05130 HOMO: -7.06408 LUMO: -1.12927 factor:1 | 1 (-2.15090) | 1 | 1 |
| G: -4614.53471 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10881.82236 HOMO: -6.70761 LUMO: -0.98505 factor:1 | 1 (-2.92196) | -1 | -1 |
| G: -4614.53471 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10882.54284 HOMO: -7.00965 LUMO: -0.42722 factor:1 | 1 (-3.64243) | -1 | -1 |
| G: -4614.53471 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10880.81886 HOMO: -5.96201 LUMO: -0.59049 factor:1 | 1 (-1.91846) | -1 | -1 |
| G: -4614.53471 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10881.55052 HOMO: -6.34570 LUMO: -1.68438 factor:1 | 1 (-2.65012) | -1 | -1 |
| G: -4614.53471 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10880.84550 HOMO: -6.97156 LUMO: -1.85854 factor:1 | 1 (-1.94510) | -1 | -1 |
| G: -4614.53471 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10880.49123 HOMO: -5.91848 LUMO: -2.51433 factor:1 | 1 (-1.59083) | -1 | -1 |
| G: -4614.53471 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10881.53378 HOMO: -6.39195 LUMO: -1.66262 factor:1 | 1 (-2.63338) | -1 | -1 |
| G: -4614.53471 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10879.79242 HOMO: -6.50352 LUMO: 0.19592 factor:1 | 1 (-0.89202) | -1 | -1 |
| G: -4614.53471 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10879.86153 HOMO: -6.45998 LUMO: 0.34831 factor:1 | 1 (-0.96113) | -1 | -1 |
| G: -4614.53471 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10879.22008 HOMO: -7.05319 LUMO: 0.23402 factor:1 | 1 (-0.31968) | -1 | -1 |
| G: -4614.53471 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10880.06957 HOMO: -6.61237 LUMO: 0.18232 factor:1 | 1 (-1.16916) | -1 | -1 |
| G: -4614.53471 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10880.01672 HOMO: -6.57427 LUMO: 0.40545 factor:1 | 1 (-1.11632) | -1 | -1 |
| G: -4614.53471 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10879.41742 HOMO: -7.26544 LUMO: 0.41089 factor:1 | 1 (-0.51702) | 1 | 1 |
| G: -4614.53471 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10879.10590 HOMO: -6.26406 LUMO: -0.85444 factor:1 | 1 (-0.20550) | -1 | -1 |
| G: -4614.53471 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10878.45985 HOMO: -6.25318 LUMO: -0.79457 factor:1 | -1 (0.44055) | -1 | -1 |
| G: -4614.53471 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10878.73659 HOMO: -6.68040 LUMO: 0.41089 factor:1 | -1 (0.16381) | -1 | -1 |
| G: -4614.53471 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10879.58439 HOMO: -6.37835 LUMO: 0.37280 factor:1 | 1 (-0.68399) | -1 | -1 |
| G: -4614.53471 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10879.55663 HOMO: -6.56067 LUMO: 0.62858 factor:1 | 1 (-0.65623) | -1 | -1 |
| G: -4614.53471 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10878.96078 HOMO: -6.74026 LUMO: -0.04082 factor:1 | 1 (-0.06038) | -1 | -1 |
| G: -4614.53471 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10879.69408 HOMO: -6.53617 LUMO: 0.35103 factor:1 | 1 (-0.79367) | -1 | -1 |
| G: -4614.53471 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10879.64460 HOMO: -6.51985 LUMO: 0.25851 factor:1 | 1 (-0.74420) | -1 | -1 |
| G: -4614.53471 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10878.32085 HOMO: -6.58788 LUMO: -1.98371 factor:1 | -1 (0.57955) | -1 | -1 |
| G: -4614.53471 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10879.62637 HOMO: -6.51441 LUMO: 0.29116 factor:1 | 1 (-0.72597) | -1 | -1 |
| G: -4614.53471 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10879.02840 HOMO: -6.81101 LUMO: 0.35647 factor:1 | 1 (-0.12800) | -1 | -1 |
| G: -4614.53471 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10879.54594 HOMO: -6.42733 LUMO: 0.10340 factor:1 | 1 (-0.64554) | -1 | -1 |
| G: -4614.53471 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10878.97493 HOMO: -6.70761 LUMO: 0.28028 factor:1 | 1 (-0.07453) | -1 | -1 |
| G: -4614.53471 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10879.73604 HOMO: -6.67495 LUMO: 0.01633 factor:1 | 1 (-0.83563) | -1 | -1 |
| G: -4614.53471 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10880.46424 HOMO: -6.75387 LUMO: 0.15510 factor:1 | 1 (-1.56384) | -1 | -1 |
| G: -4614.53471 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10880.71116 HOMO: -6.56067 LUMO: 0.35919 factor:1 | 1 (-1.81075) | -1 | -1 |
| G: -4614.53471 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10880.01063 HOMO: -7.16748 LUMO: 0.21497 factor:1 | 1 (-1.11022) | 1 | 1 |
| G: -4614.53471 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10880.63994 HOMO: -6.71849 LUMO: 0.26667 factor:1 | 1 (-1.73954) | -1 | -1 |
| G: -4614.53471 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10880.69948 HOMO: -6.69128 LUMO: 0.55783 factor:1 | 1 (-1.79908) | -1 | -1 |
| G: -4614.53471 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10880.00404 HOMO: -6.71305 LUMO: 0.45987 factor:1 | 1 (-1.10364) | -1 | -1 |
| G: -4614.53471 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10879.73473 HOMO: -5.90487 LUMO: -0.70750 factor:1 | 1 (-0.83433) | -1 | -1 |
| G: -4614.53471 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10880.08010 HOMO: -6.84638 LUMO: -0.72110 factor:1 | 1 (-1.17970) | -1 | -1 |
| G: -4614.53471 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10879.90624 HOMO: -6.66135 LUMO: -1.13471 factor:1 | 1 (-1.00584) | -1 | -1 |
| G: -4614.53471 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10880.75263 HOMO: -6.74026 LUMO: -0.64763 factor:1 | 1 (-1.85222) | -1 | -1 |
| G: -4614.53471 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10879.87917 HOMO: -6.69672 LUMO: -1.05036 factor:1 | 1 (-0.97877) | -1 | -1 |
| G: -4614.53471 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10880.72345 HOMO: -6.78924 LUMO: -1.03675 factor:1 | 1 (-1.82305) | -1 | -1 |
| G: -4614.53471 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10880.85693 HOMO: -6.81373 LUMO: -0.85988 factor:1 | 1 (-1.95653) | -1 | -1 |
| G: -4614.53471 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10879.62760 HOMO: -7.26544 LUMO: 0.91158 factor:1 | 1 (-0.72720) | 1 | 1 |
| G: -4614.53471 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10880.42783 HOMO: -6.64230 LUMO: -1.92929 factor:1 | 1 (-1.52743) | -1 | -1 |
| G: -4614.53471 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10879.44874 HOMO: -7.20830 LUMO: 0.11429 factor:1 | 1 (-0.54834) | 1 | 1 |
| G: -4614.53471 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10879.34844 HOMO: -7.17020 LUMO: 0.04898 factor:1 | 1 (-0.44804) | 1 | 1 |
| G: -4614.53471 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10879.07940 HOMO: -7.16476 LUMO: 0.04898 factor:1 | 1 (-0.17900) | 1 | 1 |
| G: -4614.53471 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10879.97435 HOMO: -6.59332 LUMO: -0.49253 factor:1 | 1 (-1.07395) | -1 | -1 |
| G: -4614.53471 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10880.24064 HOMO: -7.46953 LUMO: 0.84083 factor:1 | 1 (-1.34024) | 1 | 1 |
| G: -4614.53471 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10880.36938 HOMO: -7.39878 LUMO: 0.88709 factor:1 | 1 (-1.46898) | 1 | 1 |
| G: -4614.53471 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10880.73194 HOMO: -6.84094 LUMO: -0.61498 factor:1 | 1 (-1.83154) | -1 | -1 |
| G: -4614.53471 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10880.64862 HOMO: -6.03549 LUMO: -0.27211 factor:1 | 1 (-1.74822) | -1 | -1 |
| G: -4614.53471 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10881.19748 HOMO: -7.31170 LUMO: -0.64763 factor:1 | 1 (-2.29708) | 1 | 1 |
| G: -4614.53471 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10880.54849 HOMO: -6.88992 LUMO: -0.84627 factor:1 | 1 (-1.64808) | -1 | -1 |
| G: -4614.53471 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10879.94360 HOMO: -7.12666 LUMO: -0.09252 factor:1 | 1 (-1.04320) | 1 | 1 |
| G: -4614.53471 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10880.51586 HOMO: -6.70489 LUMO: -0.63675 factor:1 | 1 (-1.61546) | -1 | -1 |
| G: -4614.53471 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10879.53704 HOMO: -6.98788 LUMO: 0.86804 factor:1 | 1 (-0.63664) | -1 | -1 |
| G: -4614.53471 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10881.18006 HOMO: -6.80285 LUMO: -0.60954 factor:1 | 1 (-2.27966) | -1 | -1 |
| G: -4614.53471 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10880.47915 HOMO: -7.02054 LUMO: -0.74287 factor:1 | 1 (-1.57875) | -1 | -1 |
| G: -4614.53471 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10881.69240 HOMO: -7.03686 LUMO: -0.81090 factor:1 | 1 (-2.79200) | -1 | -1 |
| G: -4614.53471 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10881.26706 HOMO: -6.70489 LUMO: -1.00954 factor:1 | 1 (-2.36666) | -1 | -1 |
| G: -4614.53471 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10879.49587 HOMO: -7.69810 LUMO: 0.00544 factor:1 | 1 (-0.59547) | 1 | 1 |
| G: -4614.53471 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10879.44251 HOMO: -6.83550 LUMO: -0.11157 factor:1 | 1 (-0.54211) | -1 | -1 |
| G: -4614.53471 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10880.05922 HOMO: -6.76203 LUMO: -2.13609 factor:1 | 1 (-1.15882) | -1 | -1 |
| G: -4614.53471 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10879.71486 HOMO: -6.72121 LUMO: -2.62862 factor:1 | 1 (-0.81446) | -1 | -1 |
| G: -4614.53471 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10879.45287 HOMO: -6.48719 LUMO: -2.73474 factor:1 | 1 (-0.55247) | -1 | -1 |
| G: -4614.53471 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10879.13338 HOMO: -6.83006 LUMO: -0.00544 factor:1 | 1 (-0.23298) | -1 | -1 |
| G: -4614.53471 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10880.29022 HOMO: -6.84094 LUMO: -1.11022 factor:1 | 1 (-1.38982) | -1 | -1 |
| G: -4614.53471 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10879.91628 HOMO: -6.66951 LUMO: -1.23812 factor:1 | 1 (-1.01588) | -1 | -1 |
| G: -4614.53471 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10880.21408 HOMO: -6.78380 LUMO: -1.27894 factor:1 | 1 (-1.31368) | -1 | -1 |
| G: -4614.53471 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10880.91785 HOMO: -6.50352 LUMO: -0.56055 factor:1 | 1 (-2.01745) | -1 | -1 |
| G: -4614.53471 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10879.49511 HOMO: -7.77974 LUMO: -0.26395 factor:1 | 1 (-0.59470) | 1 | 1 |
| G: -4614.53471 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10880.89712 HOMO: -7.01510 LUMO: -1.64085 factor:1 | 1 (-1.99672) | -1 | -1 |
| G: -4614.53471 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10880.90751 HOMO: -6.59876 LUMO: -0.91158 factor:1 | 1 (-2.00711) | -1 | -1 |
| G: -4614.53471 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10879.16133 HOMO: -4.67219 LUMO: -0.67756 factor:1 | 1 (-0.26093) | -1 | -1 |
| G: -4614.53471 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10880.76441 HOMO: -6.70489 LUMO: -0.65579 factor:1 | 1 (-1.86401) | -1 | -1 |
| G: -4614.53471 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10880.88602 HOMO: -6.62325 LUMO: -0.60409 factor:1 | 1 (-1.98561) | -1 | -1 |
| G: -4614.53471 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10880.94468 HOMO: -6.20147 LUMO: 0.15238 factor:1 | 1 (-2.04428) | -1 | -1 |
| G: -4614.53471 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10880.97102 HOMO: -6.43549 LUMO: -0.07075 factor:1 | 1 (-2.07062) | -1 | -1 |
| G: -4614.53471 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10879.19954 HOMO: -7.02054 LUMO: 0.13061 factor:1 | 1 (-0.29913) | -1 | -1 |
| G: -4614.53471 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10879.06653 HOMO: -7.04503 LUMO: 0.30749 factor:1 | 1 (-0.16613) | -1 | -1 |
| G: -4614.53471 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10878.90960 HOMO: -6.74842 LUMO: -0.99594 factor:1 | 1 (-0.00920) | -1 | -1 |
| G: -4614.53471 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10879.85196 HOMO: -6.35658 LUMO: 0.41633 factor:1 | 1 (-0.95155) | -1 | -1 |
| G: -4614.53471 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10879.72390 HOMO: -6.79740 LUMO: 0.56872 factor:1 | 1 (-0.82350) | -1 | -1 |
| G: -4614.53471 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10879.87751 HOMO: -6.51713 LUMO: -0.05987 factor:1 | 1 (-0.97711) | -1 | -1 |
| G: -4614.53471 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10878.25593 HOMO: -6.68040 LUMO: 0.34558 factor:1 | -1 (0.64447) | -1 | -1 |
| G: -4614.53471 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10879.14250 HOMO: -6.39740 LUMO: 0.50069 factor:1 | 1 (-0.24210) | -1 | -1 |
| G: -4614.53471 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10878.59925 HOMO: -6.91713 LUMO: -0.97145 factor:1 | -1 (0.30115) | -1 | -1 |
| G: -4614.53471 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10878.88124 HOMO: -7.10761 LUMO: -0.27483 factor:1 | -1 (0.01916) | 1 | -1 |
| G: -4614.53471 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10879.60218 HOMO: -6.98788 LUMO: 0.40273 factor:1 | 1 (-0.70178) | -1 | -1 |
| G: -4614.53471 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10879.56433 HOMO: -6.87087 LUMO: 0.28572 factor:1 | 1 (-0.66393) | -1 | -1 |
| G: -4614.53471 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10879.94910 HOMO: -7.36612 LUMO: -0.12245 factor:1 | 1 (-1.04870) | 1 | 1 |
| G: -4614.53471 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10879.93016 HOMO: -6.72938 LUMO: 0.33742 factor:1 | 1 (-1.02976) | -1 | -1 |
| G: -4614.53471 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10879.27682 HOMO: -7.32531 LUMO: 0.07619 factor:1 | 1 (-0.37642) | 1 | 1 |
| G: -4614.53471 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10879.53364 HOMO: -6.87087 LUMO: -0.08436 factor:1 | 1 (-0.63324) | -1 | -1 |
| G: -4614.53471 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10879.85868 HOMO: -6.67495 LUMO: 0.85988 factor:1 | 1 (-0.95828) | -1 | -1 |
| G: -4614.53471 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10879.20852 HOMO: -6.96339 LUMO: 0.65307 factor:1 | 1 (-0.30811) | -1 | -1 |
| G: -4614.53471 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10879.10427 HOMO: -6.58516 LUMO: -0.78641 factor:1 | 1 (-0.20387) | -1 | -1 |
| G: -4614.53471 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10879.74243 HOMO: -6.56883 LUMO: 0.44355 factor:1 | 1 (-0.84203) | -1 | -1 |
| G: -4614.53471 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10879.58841 HOMO: -6.68312 LUMO: 0.43538 factor:1 | 1 (-0.68801) | -1 | -1 |
| G: -4614.53471 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10879.92004 HOMO: -6.81917 LUMO: 0.20681 factor:1 | 1 (-1.01964) | -1 | -1 |
| G: -4614.53471 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10879.81122 HOMO: -6.91169 LUMO: 0.08163 factor:1 | 1 (-0.91082) | -1 | -1 |
| G: -4614.53471 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10878.07557 HOMO: -4.88444 LUMO: -0.49253 factor:1 | -1 (0.82483) | -1 | -1 |
| G: -4614.53471 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10879.58890 HOMO: -6.42189 LUMO: 0.64763 factor:1 | 1 (-0.68850) | -1 | -1 |
| G: -4614.53471 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10879.65440 HOMO: -6.24501 LUMO: 0.55783 factor:1 | 1 (-0.75400) | -1 | -1 |
| G: -4614.53471 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10879.56471 HOMO: -6.41372 LUMO: 0.29388 factor:1 | 1 (-0.66431) | -1 | -1 |
| G: -4614.53471 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10877.31487 HOMO: -5.67902 LUMO: 1.77690 factor:1 | -1 (1.58553) | -1 | -1 |
| G: -4614.53471 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10879.71535 HOMO: -6.55794 LUMO: 0.05170 factor:1 | 1 (-0.81495) | -1 | -1 |
| G: -4614.53471 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10879.76746 HOMO: -6.52801 LUMO: 0.25851 factor:1 | 1 (-0.86706) | -1 | -1 |
| G: -4614.53471 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10879.13006 HOMO: -7.08857 LUMO: 0.11157 factor:1 | 1 (-0.22966) | 1 | 1 |
| G: -4614.53471 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10879.91307 HOMO: -6.58243 LUMO: 0.75648 factor:1 | 1 (-1.01267) | -1 | -1 |
| G: -4614.53471 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10879.32299 HOMO: -7.22190 LUMO: 0.45171 factor:1 | 1 (-0.42259) | 1 | 1 |
| G: -4614.53471 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10879.41889 HOMO: -6.47087 LUMO: 0.00000 factor:1 | 1 (-0.51849) | -1 | -1 |
| G: -4614.53471 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10880.83791 HOMO: -6.78652 LUMO: 1.32247 factor:1 | 1 (-1.93751) | -1 | -1 |
| G: -4614.53471 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10879.90573 HOMO: -6.74026 LUMO: 1.45309 factor:1 | 1 (-1.00532) | -1 | -1 |
| G: -4614.53471 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10879.78088 HOMO: -6.69944 LUMO: 0.76464 factor:1 | 1 (-0.88048) | -1 | -1 |
| G: -4614.53471 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10880.53009 HOMO: -6.62325 LUMO: 0.64763 factor:1 | 1 (-1.62969) | -1 | -1 |
| G: -4614.53471 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10879.81930 HOMO: -6.45182 LUMO: 0.49253 factor:1 | 1 (-0.91890) | -1 | -1 |
| G: -4614.53471 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10879.93046 HOMO: -7.14843 LUMO: 0.62586 factor:1 | 1 (-1.03006) | 1 | 1 |
| G: -4614.53471 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10880.26116 HOMO: -6.87087 LUMO: 1.53200 factor:1 | 1 (-1.36076) | -1 | -1 |
| G: -4614.53471 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10880.51091 HOMO: -6.54978 LUMO: 0.45171 factor:1 | 1 (-1.61051) | -1 | -1 |
| G: -4614.53471 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10880.65529 HOMO: -6.63686 LUMO: 0.80001 factor:1 | 1 (-1.75489) | -1 | -1 |
| G: -4614.53471 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10881.11329 HOMO: -7.00693 LUMO: 1.56193 factor:1 | 1 (-2.21288) | -1 | -1 |
| G: -4614.53471 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10877.59221 HOMO: -6.02460 LUMO: 1.72792 factor:1 | -1 (1.30819) | -1 | -1 |
| G: -4614.53471 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10877.85899 HOMO: -6.36746 LUMO: -1.20002 factor:1 | -1 (1.04141) | -1 | -1 |
| G: -4614.53471 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10880.07819 HOMO: -7.26816 LUMO: -1.06397 factor:1 | 1 (-1.17779) | 1 | 1 |
| G: -4614.53471 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10880.27161 HOMO: -7.34707 LUMO: -1.09662 factor:1 | 1 (-1.37121) | 1 | 1 |
| G: -4614.53471 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10881.02615 HOMO: -7.93212 LUMO: -0.13606 factor:1 | 1 (-2.12575) | 1 | 1 |
| G: -4614.53471 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10879.55630 HOMO: -6.80285 LUMO: 0.58504 factor:1 | 1 (-0.65590) | -1 | -1 |
| G: -4614.53471 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10878.62050 HOMO: -7.12938 LUMO: 0.32926 factor:1 | -1 (0.27990) | 1 | -1 |
| G: -4614.53471 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10880.34865 HOMO: -6.86815 LUMO: -1.30070 factor:1 | 1 (-1.44824) | -1 | -1 |
| G: -4614.53471 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10879.94260 HOMO: -6.99333 LUMO: -1.03947 factor:1 | 1 (-1.04220) | -1 | -1 |
| G: -4614.53471 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10879.20081 HOMO: -7.56749 LUMO: -0.11157 factor:1 | 1 (-0.30041) | 1 | 1 |
| G: -4614.53471 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10879.37668 HOMO: -7.57293 LUMO: -0.07891 factor:1 | 1 (-0.47628) | 1 | 1 |
| G: -4614.53471 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10879.54640 HOMO: -7.30626 LUMO: 0.27211 factor:1 | 1 (-0.64600) | 1 | 1 |
| G: -4614.53471 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10880.15651 HOMO: -7.77974 LUMO: 0.27211 factor:1 | 1 (-1.25610) | 1 | 1 |
| G: -4614.53471 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10879.94763 HOMO: -7.11578 LUMO: 0.19864 factor:1 | 1 (-1.04723) | 1 | 1 |
| G: -4614.53471 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10880.25153 HOMO: -7.71171 LUMO: 0.57688 factor:1 | 1 (-1.35113) | 1 | 1 |
| G: -4614.53471 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10880.06494 HOMO: -7.83688 LUMO: 0.37824 factor:1 | 1 (-1.16454) | 1 | 1 |
| G: -4614.53471 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10880.56337 HOMO: -6.94979 LUMO: -1.66534 factor:1 | 1 (-1.66297) | -1 | -1 |
| G: -4614.53471 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10880.48299 HOMO: -6.97156 LUMO: -1.13199 factor:1 | 1 (-1.58259) | -1 | -1 |
| G: -4614.53471 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10880.39425 HOMO: -6.91441 LUMO: -1.08301 factor:1 | 1 (-1.49385) | -1 | -1 |
| G: -4614.53471 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10880.51858 HOMO: -6.71849 LUMO: -0.74831 factor:1 | 1 (-1.61818) | -1 | -1 |
| G: -4614.53471 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10879.25475 HOMO: -7.09401 LUMO: -1.77690 factor:1 | 1 (-0.35435) | -1 | -1 |
| G: -4614.53471 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10879.23404 HOMO: -6.97156 LUMO: -1.45037 factor:1 | 1 (-0.33364) | -1 | -1 |
| G: -4614.53471 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10880.64163 HOMO: -7.22462 LUMO: -1.11295 factor:1 | 1 (-1.74123) | 1 | 1 |
| G: -4614.53471 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10879.07741 HOMO: -7.85321 LUMO: 0.16599 factor:1 | 1 (-0.17701) | 1 | 1 |
| G: -4614.53471 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10879.42958 HOMO: -7.71987 LUMO: 0.55511 factor:1 | 1 (-0.52918) | 1 | 1 |
| G: -4614.53471 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10879.06049 HOMO: -7.63551 LUMO: 0.14422 factor:1 | 1 (-0.16008) | 1 | 1 |
| G: -4614.53471 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10880.00088 HOMO: -6.98788 LUMO: -0.80546 factor:1 | 1 (-1.10048) | -1 | -1 |
| G: -4614.53471 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10879.97819 HOMO: -6.98788 LUMO: -1.16737 factor:1 | 1 (-1.07779) | -1 | -1 |
| G: -4614.53471 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10879.20841 HOMO: -6.56611 LUMO: -1.60819 factor:1 | 1 (-0.30801) | -1 | -1 |
| G: -4614.53471 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10879.29230 HOMO: -6.95251 LUMO: 0.66396 factor:1 | 1 (-0.39190) | -1 | -1 |
| G: -4614.53471 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10879.64229 HOMO: -7.35252 LUMO: 0.49797 factor:1 | 1 (-0.74189) | 1 | 1 |
| G: -4614.53471 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10879.59239 HOMO: -6.90897 LUMO: -0.81090 factor:1 | 1 (-0.69199) | -1 | -1 |
| G: -4614.53471 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10879.88820 HOMO: -7.04503 LUMO: -1.08301 factor:1 | 1 (-0.98780) | -1 | -1 |
| G: -4614.53471 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10879.59497 HOMO: -6.92530 LUMO: -1.29526 factor:1 | 1 (-0.69457) | -1 | -1 |
| G: -4614.53471 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10879.31301 HOMO: -6.93074 LUMO: -1.25444 factor:1 | 1 (-0.41261) | -1 | -1 |
| G: -4614.53471 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10880.45431 HOMO: -6.73482 LUMO: -0.62042 factor:1 | 1 (-1.55391) | -1 | -1 |
| G: -4614.53471 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10879.51260 HOMO: -7.67633 LUMO: 0.59593 factor:1 | 1 (-0.61220) | 1 | 1 |
| G: -4614.53471 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10879.15553 HOMO: -7.39061 LUMO: -0.19320 factor:1 | 1 (-0.25513) | 1 | 1 |
| G: -4614.53471 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10879.43796 HOMO: -7.55388 LUMO: -0.20136 factor:1 | 1 (-0.53756) | 1 | 1 |
| G: -4614.53471 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10880.81295 HOMO: -7.14027 LUMO: -0.99866 factor:1 | 1 (-1.91255) | 1 | 1 |
| G: -4614.53471 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10881.54488 HOMO: -6.75931 LUMO: -0.73199 factor:1 | 1 (-2.64448) | -1 | -1 |
| G: -4614.53471 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10879.60308 HOMO: -5.45044 LUMO: -0.18776 factor:1 | 1 (-0.70268) | -1 | -1 |
| G: -4614.53471 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10881.76492 HOMO: -6.70761 LUMO: -0.84083 factor:1 | 1 (-2.86452) | -1 | -1 |
| G: -4614.53471 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10880.46353 HOMO: -6.05453 LUMO: -1.06669 factor:1 | 1 (-1.56313) | -1 | -1 |
| G: -4614.53471 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10880.47140 HOMO: -6.86815 LUMO: -0.98233 factor:1 | 1 (-1.57099) | -1 | -1 |
| G: -4614.53471 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10880.58405 HOMO: -6.73210 LUMO: -0.95240 factor:1 | 1 (-1.68365) | -1 | -1 |
| G: -4614.53471 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10880.56745 HOMO: -5.89671 LUMO: -1.05036 factor:1 | 1 (-1.66705) | -1 | -1 |
| G: -4614.53471 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10880.24456 HOMO: -7.61102 LUMO: 0.33470 factor:1 | 1 (-1.34416) | 1 | 1 |
| G: -4614.53471 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10880.22448 HOMO: -7.51034 LUMO: 0.23674 factor:1 | 1 (-1.32408) | 1 | 1 |
| G: -4614.53471 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10880.20285 HOMO: -7.41510 LUMO: 0.62858 factor:1 | 1 (-1.30245) | 1 | 1 |
| G: -4614.53471 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10880.68778 HOMO: -6.76203 LUMO: -1.72792 factor:1 | 1 (-1.78738) | -1 | -1 |
| G: -4614.53471 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10881.15508 HOMO: -6.60420 LUMO: -0.45715 factor:1 | 1 (-2.25468) | -1 | -1 |
| G: -4614.53471 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10880.46307 HOMO: -6.59060 LUMO: -0.58232 factor:1 | 1 (-1.56267) | -1 | -1 |
| G: -4614.53471 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10881.43764 HOMO: -7.43687 LUMO: -0.76736 factor:1 | 1 (-2.53724) | 1 | 1 |
| G: -4614.53471 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10880.52329 HOMO: -6.08719 LUMO: -0.48708 factor:1 | 1 (-1.62289) | -1 | -1 |
| G: -4614.53471 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10880.94444 HOMO: -5.88854 LUMO: -0.05714 factor:1 | 1 (-2.04404) | -1 | -1 |
| G: -4614.53471 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10880.42655 HOMO: -7.34435 LUMO: -0.71838 factor:1 | 1 (-1.52615) | 1 | 1 |
| G: -4614.53471 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10880.62571 HOMO: -7.46408 LUMO: -0.63130 factor:1 | 1 (-1.72531) | 1 | 1 |
| G: -4614.53471 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10879.90771 HOMO: -7.00965 LUMO: -1.24900 factor:1 | 1 (-1.00731) | -1 | -1 |
| G: -4614.53471 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10880.11193 HOMO: -6.91169 LUMO: -0.88981 factor:1 | 1 (-1.21153) | -1 | -1 |
| G: -4614.53471 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10881.04245 HOMO: -6.78652 LUMO: -0.82178 factor:1 | 1 (-2.14205) | -1 | -1 |
| G: -4614.53471 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10879.50732 HOMO: -7.80423 LUMO: 0.87076 factor:1 | 1 (-0.60692) | 1 | 1 |
| G: -4614.53471 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10881.28017 HOMO: -6.97700 LUMO: -1.00954 factor:1 | 1 (-2.37977) | -1 | -1 |
| G: -4614.53471 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10880.84770 HOMO: -6.92530 LUMO: -0.88165 factor:1 | 1 (-1.94730) | -1 | -1 |
| G: -4614.53471 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10880.23229 HOMO: -7.14571 LUMO: -1.04492 factor:1 | 1 (-1.33189) | 1 | 1 |
| G: -4614.53471 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10879.88377 HOMO: -7.49674 LUMO: 0.34558 factor:1 | 1 (-0.98337) | 1 | 1 |
| G: -4614.53471 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10878.60995 HOMO: -6.44094 LUMO: -1.20819 factor:1 | -1 (0.29045) | -1 | -1 |
| G: -4614.53471 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10878.64532 HOMO: -6.47359 LUMO: -1.14016 factor:1 | -1 (0.25508) | -1 | -1 |
| G: -4614.53471 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10878.66734 HOMO: -6.61237 LUMO: -0.87076 factor:1 | -1 (0.23307) | -1 | -1 |
| G: -4614.53471 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10878.58159 HOMO: -6.73754 LUMO: -1.09662 factor:1 | -1 (0.31881) | -1 | -1 |
| G: -4614.53471 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10878.91431 HOMO: -6.97700 LUMO: 0.13061 factor:1 | 1 (-0.01391) | -1 | -1 |
| G: -4614.53471 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10879.50077 HOMO: -6.82734 LUMO: 0.59865 factor:1 | 1 (-0.60036) | -1 | -1 |
| G: -4614.53471 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10879.54795 HOMO: -6.86543 LUMO: -0.91430 factor:1 | 1 (-0.64755) | -1 | -1 |
| G: -4614.53471 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10879.58575 HOMO: -6.74298 LUMO: 0.28028 factor:1 | 1 (-0.68535) | -1 | -1 |
| G: -4614.53471 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10879.58392 HOMO: -6.75387 LUMO: 0.19592 factor:1 | 1 (-0.68352) | -1 | -1 |
| G: -4614.53471 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10879.78978 HOMO: -7.05591 LUMO: 0.10612 factor:1 | 1 (-0.88938) | -1 | -1 |
| G: -4614.53471 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10879.85756 HOMO: -6.86543 LUMO: 0.49253 factor:1 | 1 (-0.95716) | -1 | -1 |
| G: -4614.53471 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10879.53758 HOMO: -6.11440 LUMO: -1.12655 factor:1 | 1 (-0.63718) | -1 | -1 |
| G: -4614.53471 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10879.63963 HOMO: -6.77291 LUMO: -1.02859 factor:1 | 1 (-0.73922) | -1 | -1 |
| G: -4614.53471 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10880.52517 HOMO: -6.54978 LUMO: 0.29116 factor:1 | 1 (-1.62476) | -1 | -1 |
| G: -4614.53471 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10880.51382 HOMO: -7.18108 LUMO: 0.00000 factor:1 | 1 (-1.61342) | 1 | 1 |
| G: -4614.53471 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10878.94029 HOMO: -6.86271 LUMO: -1.15376 factor:1 | 1 (-0.03989) | -1 | -1 |
| G: -4614.53471 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10878.65982 HOMO: -6.78108 LUMO: -1.22723 factor:1 | -1 (0.24058) | -1 | -1 |
| G: -4614.53471 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10879.42629 HOMO: -6.40828 LUMO: 0.02449 factor:1 | 1 (-0.52589) | -1 | -1 |
| G: -4614.53471 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10879.20696 HOMO: -6.43821 LUMO: 0.09796 factor:1 | 1 (-0.30656) | -1 | -1 |
| G: -4614.53471 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10878.57005 HOMO: -6.99877 LUMO: 0.40545 factor:1 | -1 (0.33035) | -1 | -1 |
| G: -4614.53471 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10879.48917 HOMO: -6.68856 LUMO: 0.19320 factor:1 | 1 (-0.58877) | -1 | -1 |
| G: -4614.53471 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10878.91292 HOMO: -7.11034 LUMO: 0.31293 factor:1 | 1 (-0.01252) | 1 | 1 |
| G: -4614.53471 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10878.93700 HOMO: -6.92530 LUMO: -0.85444 factor:1 | 1 (-0.03660) | -1 | -1 |
| G: -4614.53471 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10878.90720 HOMO: -6.60148 LUMO: -0.59865 factor:1 | 1 (-0.00680) | -1 | -1 |
| G: -4614.53471 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10879.84322 HOMO: -6.72938 LUMO: 0.30749 factor:1 | 1 (-0.94282) | -1 | -1 |
| G: -4614.53471 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10879.26150 HOMO: -7.31170 LUMO: 0.06803 factor:1 | 1 (-0.36110) | 1 | 1 |
| G: -4614.53471 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10879.86559 HOMO: -7.09129 LUMO: -0.04626 factor:1 | 1 (-0.96519) | 1 | 1 |
| G: -4614.53471 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10879.08220 HOMO: -6.38379 LUMO: -0.76736 factor:1 | 1 (-0.18180) | -1 | -1 |
| G: -4614.53471 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10879.19630 HOMO: -6.13617 LUMO: -0.63947 factor:1 | 1 (-0.29590) | -1 | -1 |
| G: -4614.53471 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10879.60210 HOMO: -6.92258 LUMO: 0.37007 factor:1 | 1 (-0.70170) | -1 | -1 |
| G: -4614.53471 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10880.34840 HOMO: -6.35930 LUMO: 0.41361 factor:1 | 1 (-1.44800) | -1 | -1 |
| G: -4614.53471 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10880.04023 HOMO: -6.60420 LUMO: 0.26667 factor:1 | 1 (-1.13983) | -1 | -1 |
| G: -4614.53471 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10876.94458 HOMO: -6.04909 LUMO: 1.82588 factor:1 | -1 (1.95582) | -1 | -1 |
| G: -4614.53471 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10877.86128 HOMO: -6.69672 LUMO: 1.72520 factor:1 | -1 (1.03912) | -1 | -1 |
| G: -4614.53471 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10879.55832 HOMO: -6.50080 LUMO: 0.29116 factor:1 | 1 (-0.65792) | -1 | -1 |
| G: -4614.53471 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10879.35173 HOMO: -6.60692 LUMO: -0.43266 factor:1 | 1 (-0.45133) | -1 | -1 |
| G: -4614.53471 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10880.42671 HOMO: -6.93890 LUMO: 0.39729 factor:1 | 1 (-1.52631) | -1 | -1 |
| G: -4614.53471 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10879.20291 HOMO: -6.52801 LUMO: -0.47076 factor:1 | 1 (-0.30251) | -1 | -1 |
| G: -4614.53471 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10879.47666 HOMO: -6.41100 LUMO: 0.30477 factor:1 | 1 (-0.57626) | -1 | -1 |
| G: -4614.53471 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10878.64595 HOMO: -6.37291 LUMO: -0.80001 factor:1 | -1 (0.25445) | -1 | -1 |
| G: -4614.53471 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10880.72422 HOMO: -6.51985 LUMO: 1.44765 factor:1 | 1 (-1.82382) | -1 | -1 |
| G: -4614.53471 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10880.38818 HOMO: -6.64774 LUMO: 0.04626 factor:1 | 1 (-1.48778) | -1 | -1 |
| G: -4614.53471 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10880.56582 HOMO: -6.65863 LUMO: 0.29933 factor:1 | 1 (-1.66542) | -1 | -1 |
| G: -4614.53471 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10879.82534 HOMO: -7.09673 LUMO: 0.28300 factor:1 | 1 (-0.92494) | 1 | 1 |
| G: -4614.53471 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10879.59571 HOMO: -6.57155 LUMO: -1.11567 factor:1 | 1 (-0.69531) | -1 | -1 |
| G: -4614.53471 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10879.80956 HOMO: -6.38379 LUMO: -0.60681 factor:1 | 1 (-0.90916) | -1 | -1 |
| G: -4614.53471 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10880.39275 HOMO: -6.60148 LUMO: 0.18232 factor:1 | 1 (-1.49235) | -1 | -1 |
| G: -4614.53471 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10879.97639 HOMO: -6.96067 LUMO: -0.52246 factor:1 | 1 (-1.07599) | -1 | -1 |
| G: -4614.53471 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10879.68199 HOMO: -6.57427 LUMO: -0.84627 factor:1 | 1 (-0.78159) | -1 | -1 |
| G: -4614.53471 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10879.60150 HOMO: -6.59332 LUMO: -0.98233 factor:1 | 1 (-0.70110) | -1 | -1 |
| G: -4614.53471 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10879.38144 HOMO: -6.20692 LUMO: -0.27483 factor:1 | 1 (-0.48104) | -1 | -1 |
| G: -4614.53471 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10879.41233 HOMO: -6.81373 LUMO: 0.74559 factor:1 | 1 (-0.51193) | -1 | -1 |
| G: -4614.53471 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10879.92521 HOMO: -6.60420 LUMO: 0.54695 factor:1 | 1 (-1.02481) | -1 | -1 |
| G: -4614.53471 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10879.21720 HOMO: -6.58788 LUMO: -0.31021 factor:1 | 1 (-0.31679) | -1 | -1 |
| G: -4614.53471 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10880.24451 HOMO: -6.72938 LUMO: 0.64763 factor:1 | 1 (-1.34411) | -1 | -1 |
| G: -4614.53471 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10879.70782 HOMO: -6.86815 LUMO: 0.32109 factor:1 | 1 (-0.80742) | -1 | -1 |
| G: -4614.53471 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10880.53050 HOMO: -6.63141 LUMO: 0.18776 factor:1 | 1 (-1.63010) | -1 | -1 |
| G: -4614.53471 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10879.90812 HOMO: -7.18653 LUMO: 0.09524 factor:1 | 1 (-1.00772) | 1 | 1 |
| G: -4614.53471 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10880.41578 HOMO: -6.83550 LUMO: 0.03537 factor:1 | 1 (-1.51537) | -1 | -1 |
| G: -4614.53471 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10880.51580 HOMO: -7.47769 LUMO: 0.40817 factor:1 | 1 (-1.61540) | 1 | 1 |
| G: -4614.53471 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10879.86202 HOMO: -6.57971 LUMO: -0.63675 factor:1 | 1 (-0.96162) | -1 | -1 |
| G: -4614.53471 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10879.91764 HOMO: -6.74842 LUMO: -0.16327 factor:1 | 1 (-1.01724) | -1 | -1 |
| G: -4614.53471 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10879.68452 HOMO: -7.07224 LUMO: 0.61770 factor:1 | 1 (-0.78412) | 1 | 1 |
| G: -4614.53471 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10879.41418 HOMO: -6.83006 LUMO: 0.54695 factor:1 | 1 (-0.51378) | -1 | -1 |
| G: -4614.53471 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10879.75214 HOMO: -6.60148 LUMO: 1.23540 factor:1 | 1 (-0.85174) | -1 | -1 |
| G: -4614.53471 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10880.21536 HOMO: -6.99061 LUMO: 0.41089 factor:1 | 1 (-1.31496) | -1 | -1 |
| G: -4614.53471 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10880.63504 HOMO: -6.63686 LUMO: 0.85172 factor:1 | 1 (-1.73464) | -1 | -1 |
| G: -4614.53471 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10880.05253 HOMO: -6.50624 LUMO: 0.12517 factor:1 | 1 (-1.15213) | -1 | -1 |
| G: -4614.53471 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10880.05484 HOMO: -6.35658 LUMO: 0.36463 factor:1 | 1 (-1.15444) | -1 | -1 |
| G: -4614.53471 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10880.24804 HOMO: -6.34570 LUMO: 0.65035 factor:1 | 1 (-1.34764) | -1 | -1 |
| G: -4614.53471 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10880.77129 HOMO: -6.63141 LUMO: 1.25717 factor:1 | 1 (-1.87089) | -1 | -1 |
| G: -4614.53471 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10880.74566 HOMO: -6.91441 LUMO: 1.32792 factor:1 | 1 (-1.84526) | -1 | -1 |
| G: -4614.53471 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10880.47001 HOMO: -7.15387 LUMO: 0.64219 factor:1 | 1 (-1.56961) | 1 | 1 |
| G: -4614.53471 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10880.52380 HOMO: -7.17836 LUMO: 0.60409 factor:1 | 1 (-1.62340) | 1 | 1 |
| G: -4614.53471 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10880.18570 HOMO: -6.92258 LUMO: 0.49525 factor:1 | 1 (-1.28530) | -1 | -1 |
| G: -4614.53471 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10880.75717 HOMO: -6.31032 LUMO: 0.48708 factor:1 | 1 (-1.85677) | -1 | -1 |
| G: -4614.53471 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10880.74797 HOMO: -6.49808 LUMO: 0.31021 factor:1 | 1 (-1.84757) | -1 | -1 |
| G: -4614.53471 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10878.30395 HOMO: -6.48447 LUMO: 0.37552 factor:1 | -1 (0.59645) | -1 | -1 |
| G: -4614.53471 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10877.90580 HOMO: -6.66135 LUMO: -1.08301 factor:1 | -1 (0.99460) | -1 | -1 |
| G: -4614.53471 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10877.74533 HOMO: -6.33481 LUMO: -0.51974 factor:1 | -1 (1.15507) | -1 | -1 |
| G: -4614.53471 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10877.76207 HOMO: -6.76475 LUMO: -0.15238 factor:1 | -1 (1.13833) | -1 | -1 |
| G: -4614.53471 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10878.02153 HOMO: -6.93346 LUMO: -0.10885 factor:1 | -1 (0.87887) | -1 | -1 |
| G: -4614.53471 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10879.19994 HOMO: -7.19741 LUMO: 0.73199 factor:1 | 1 (-0.29954) | 1 | 1 |
| G: -4614.53471 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10879.78828 HOMO: -6.82734 LUMO: 0.88437 factor:1 | 1 (-0.88788) | -1 | -1 |
| G: -4614.53471 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10879.85481 HOMO: -7.01237 LUMO: 0.02721 factor:1 | 1 (-0.95441) | -1 | -1 |
| G: -4614.53471 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10876.35469 HOMO: -6.39195 LUMO: 1.46941 factor:1 | -1 (2.54571) | -1 | -1 |
| G: -4614.53471 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10876.43739 HOMO: -6.53890 LUMO: 1.32792 factor:1 | -1 (2.46301) | -1 | -1 |
| G: -4614.53471 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10876.93460 HOMO: -6.82734 LUMO: 1.98099 factor:1 | -1 (1.96580) | -1 | -1 |
| G: -4614.53471 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10876.69715 HOMO: -6.74570 LUMO: 1.68983 factor:1 | -1 (2.20325) | -1 | -1 |
| G: -4614.53471 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10877.30192 HOMO: -6.41100 LUMO: 1.39050 factor:1 | -1 (1.59848) | -1 | -1 |
| G: -4614.53471 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10877.05207 HOMO: -5.92664 LUMO: 1.65989 factor:1 | -1 (1.84833) | -1 | -1 |
| G: -4614.53471 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10876.81228 HOMO: -6.07630 LUMO: 1.54833 factor:1 | -1 (2.08812) | -1 | -1 |
| G: -4614.53471 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10879.74970 HOMO: -6.45998 LUMO: 0.68573 factor:1 | 1 (-0.84929) | -1 | -1 |
| G: -4614.53471 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10879.34906 HOMO: -6.52801 LUMO: 0.41361 factor:1 | 1 (-0.44866) | -1 | -1 |
| G: -4614.53471 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10879.52809 HOMO: -6.77564 LUMO: 0.42178 factor:1 | 1 (-0.62769) | -1 | -1 |
| G: -4614.53471 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10877.78141 HOMO: -6.56339 LUMO: 1.65717 factor:1 | -1 (1.11899) | -1 | -1 |
| G: -4614.53471 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10877.76103 HOMO: -5.85861 LUMO: 1.90752 factor:1 | -1 (1.13937) | -1 | -1 |
| G: -4614.53471 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10880.12410 HOMO: -6.77019 LUMO: -2.48440 factor:1 | 1 (-1.22370) | -1 | -1 |
| G: -4614.53471 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10880.31716 HOMO: -6.53890 LUMO: -1.82588 factor:1 | 1 (-1.41676) | -1 | -1 |
| G: -4614.53471 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10881.14379 HOMO: -6.50352 LUMO: -1.66806 factor:1 | 1 (-2.24339) | -1 | -1 |
| G: -4614.53471 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10877.68778 HOMO: -6.90625 LUMO: 0.43538 factor:1 | -1 (1.21262) | -1 | -1 |
| G: -4614.53471 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10878.47430 HOMO: -6.85455 LUMO: 0.53062 factor:1 | -1 (0.42610) | -1 | -1 |
| G: -4614.53471 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10878.74992 HOMO: -6.49536 LUMO: 0.31021 factor:1 | -1 (0.15048) | -1 | -1 |
| G: -4614.53471 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10877.48522 HOMO: -4.97696 LUMO: -0.09252 factor:1 | -1 (1.41518) | -1 | -1 |
| G: -4614.53471 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10877.59126 HOMO: -5.31166 LUMO: 0.34286 factor:1 | -1 (1.30914) | -1 | -1 |
| G: -4614.53471 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10879.50477 HOMO: -6.42461 LUMO: 0.74287 factor:1 | 1 (-0.60436) | -1 | -1 |
| G: -4614.53471 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10879.55600 HOMO: -6.59604 LUMO: 0.62858 factor:1 | 1 (-0.65560) | -1 | -1 |
| G: -4614.53471 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10879.41178 HOMO: -6.45998 LUMO: -0.61770 factor:1 | 1 (-0.51138) | -1 | -1 |
| G: -4614.53471 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10879.35693 HOMO: -6.75659 LUMO: -0.34014 factor:1 | 1 (-0.45653) | -1 | -1 |
| G: -4614.53471 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10879.41565 HOMO: -6.63958 LUMO: 0.36191 factor:1 | 1 (-0.51525) | -1 | -1 |
| G: -4614.53471 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10879.71421 HOMO: -5.92936 LUMO: -0.67484 factor:1 | 1 (-0.81381) | -1 | -1 |
| G: -4614.53471 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10878.17388 HOMO: -5.67630 LUMO: 1.80956 factor:1 | -1 (0.72652) | -1 | -1 |
| G: -4614.53471 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10878.50336 HOMO: -6.50352 LUMO: -0.78369 factor:1 | -1 (0.39704) | -1 | -1 |
| G: -4614.53471 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10878.50921 HOMO: -6.35930 LUMO: -0.75648 factor:1 | -1 (0.39119) | -1 | -1 |
| G: -4614.53471 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10879.32376 HOMO: -6.74298 LUMO: 0.48980 factor:1 | 1 (-0.42335) | -1 | -1 |
| G: -4614.53471 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10878.78184 HOMO: -6.85183 LUMO: 0.15510 factor:1 | -1 (0.11856) | -1 | -1 |
| G: -4614.53471 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10879.25809 HOMO: -6.90897 LUMO: 0.26123 factor:1 | 1 (-0.35769) | -1 | -1 |
| G: -4614.53471 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10879.56392 HOMO: -6.85999 LUMO: 0.47892 factor:1 | 1 (-0.66352) | -1 | -1 |
| G: -4614.53471 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10879.53867 HOMO: -6.69944 LUMO: 0.57416 factor:1 | 1 (-0.63827) | -1 | -1 |
| G: -4614.53471 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10878.23459 HOMO: -6.74026 LUMO: 0.69933 factor:1 | -1 (0.66581) | -1 | -1 |
| G: -4614.53471 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10879.16313 HOMO: -6.52801 LUMO: 0.75376 factor:1 | 1 (-0.26273) | -1 | -1 |
| G: -4614.53471 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10880.68988 HOMO: -7.05863 LUMO: 0.44627 factor:1 | 1 (-1.78948) | -1 | -1 |
| G: -4614.53471 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10880.40454 HOMO: -6.96339 LUMO: 0.48164 factor:1 | 1 (-1.50414) | -1 | -1 |
| G: -4614.53471 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10880.08595 HOMO: -6.95795 LUMO: 0.44355 factor:1 | 1 (-1.18555) | -1 | -1 |
| G: -4614.53471 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10879.20615 HOMO: -6.36746 LUMO: 0.58777 factor:1 | 1 (-0.30575) | -1 | -1 |
| G: -4614.53471 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10878.70614 HOMO: -6.69400 LUMO: 0.40545 factor:1 | -1 (0.19426) | -1 | -1 |
| G: -4614.53471 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10879.39094 HOMO: -6.30760 LUMO: -0.66668 factor:1 | 1 (-0.49054) | -1 | -1 |
| G: -4614.53471 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10879.31488 HOMO: -6.53617 LUMO: -0.64491 factor:1 | 1 (-0.41448) | -1 | -1 |
| G: -4614.53471 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10879.59456 HOMO: -6.80829 LUMO: 0.17415 factor:1 | 1 (-0.69416) | -1 | -1 |
| G: -4614.53471 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10879.44904 HOMO: -6.80285 LUMO: 0.73471 factor:1 | 1 (-0.54864) | -1 | -1 |
| G: -4614.53471 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10879.45290 HOMO: -6.43821 LUMO: 0.21769 factor:1 | 1 (-0.55250) | -1 | -1 |
| G: -4614.53471 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10879.66335 HOMO: -6.98788 LUMO: 0.10885 factor:1 | 1 (-0.76295) | -1 | -1 |
| G: -4614.53471 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10879.82308 HOMO: -7.15115 LUMO: 0.40817 factor:1 | 1 (-0.92268) | 1 | 1 |
| G: -4614.53471 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10879.47772 HOMO: -6.00011 LUMO: -0.98505 factor:1 | 1 (-0.57732) | -1 | -1 |
| G: -4614.53471 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10879.47957 HOMO: -6.16882 LUMO: -0.77825 factor:1 | 1 (-0.57917) | -1 | -1 |
| G: -4614.53471 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10880.37518 HOMO: -6.30760 LUMO: 0.34831 factor:1 | 1 (-1.47478) | -1 | -1 |
| G: -4614.53471 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10880.55978 HOMO: -6.64502 LUMO: 0.63403 factor:1 | 1 (-1.65938) | -1 | -1 |
| G: -4614.53471 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10880.62587 HOMO: -6.93618 LUMO: 0.96600 factor:1 | 1 (-1.72547) | -1 | -1 |
| G: -4614.53471 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10880.23183 HOMO: -6.45182 LUMO: 0.16327 factor:1 | 1 (-1.33143) | -1 | -1 |
| G: -4614.53471 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10879.00046 HOMO: -6.99605 LUMO: 0.20953 factor:1 | 1 (-0.10006) | -1 | -1 |
| G: -4614.53471 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10879.18819 HOMO: -6.72665 LUMO: 0.32654 factor:1 | 1 (-0.28779) | -1 | -1 |
| G: -4614.53471 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10879.30430 HOMO: -6.38379 LUMO: 0.45443 factor:1 | 1 (-0.40390) | -1 | -1 |
| G: -4614.53471 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10878.91907 HOMO: -6.65318 LUMO: 0.04354 factor:1 | 1 (-0.01867) | -1 | -1 |
| G: -4614.53471 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10878.61090 HOMO: -6.94707 LUMO: -1.68438 factor:1 | -1 (0.28950) | -1 | -1 |
| G: -4614.53471 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10879.26435 HOMO: -6.71849 LUMO: 0.15783 factor:1 | 1 (-0.36395) | -1 | -1 |
| G: -4614.53471 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10878.54363 HOMO: -6.97156 LUMO: 0.43266 factor:1 | -1 (0.35677) | -1 | -1 |
| G: -4614.53471 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10879.10555 HOMO: -6.91441 LUMO: -0.54695 factor:1 | 1 (-0.20515) | -1 | -1 |
| G: -4614.53471 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10878.71710 HOMO: -6.74842 LUMO: -0.76192 factor:1 | -1 (0.18330) | -1 | -1 |
| G: -4614.53471 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10879.40977 HOMO: -6.70489 LUMO: 0.19048 factor:1 | 1 (-0.50937) | -1 | -1 |
| G: -4614.53471 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10878.80957 HOMO: -7.25728 LUMO: 0.33470 factor:1 | -1 (0.09083) | 1 | -1 |
| G: -4614.53471 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10878.49321 HOMO: -6.96339 LUMO: 0.55511 factor:1 | -1 (0.40719) | -1 | -1 |
| G: -4614.53471 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10879.47897 HOMO: -6.77564 LUMO: 0.72382 factor:1 | 1 (-0.57857) | -1 | -1 |
| G: -4614.53471 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10879.03129 HOMO: -6.75387 LUMO: 0.39729 factor:1 | 1 (-0.13089) | -1 | -1 |
| G: -4614.53471 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10879.06976 HOMO: -7.00149 LUMO: 0.06531 factor:1 | 1 (-0.16936) | -1 | -1 |
| G: -4614.53471 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10879.94230 HOMO: -7.09945 LUMO: 0.33470 factor:1 | 1 (-1.04190) | 1 | 1 |
| G: -4614.53471 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10879.96622 HOMO: -7.20830 LUMO: 0.59593 factor:1 | 1 (-1.06582) | 1 | 1 |
| G: -4614.53471 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10880.53983 HOMO: -6.40556 LUMO: 0.56600 factor:1 | 1 (-1.63943) | -1 | -1 |
| G: -4614.53471 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10880.57306 HOMO: -6.77291 LUMO: 0.73471 factor:1 | 1 (-1.67266) | -1 | -1 |
| G: -4614.53471 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10880.63475 HOMO: -6.65046 LUMO: 0.09796 factor:1 | 1 (-1.73434) | -1 | -1 |
| G: -4614.53471 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10879.80197 HOMO: -6.95795 LUMO: 0.22313 factor:1 | 1 (-0.90157) | -1 | -1 |
| G: -4614.53471 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10879.85870 HOMO: -6.85727 LUMO: 0.04626 factor:1 | 1 (-0.95830) | -1 | -1 |
| G: -4614.53471 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10880.45235 HOMO: -7.27360 LUMO: 0.42178 factor:1 | 1 (-1.55195) | 1 | 1 |
| G: -4614.53471 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10880.09689 HOMO: -6.78924 LUMO: -0.13334 factor:1 | 1 (-1.19648) | -1 | -1 |
| G: -4614.53471 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10880.54759 HOMO: -6.63141 LUMO: 0.38368 factor:1 | 1 (-1.64719) | -1 | -1 |
| G: -4614.53471 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10879.84866 HOMO: -6.92258 LUMO: 0.39184 factor:1 | 1 (-0.94826) | -1 | -1 |
| G: -4614.53471 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10879.69018 HOMO: -6.19331 LUMO: -0.46804 factor:1 | 1 (-0.78978) | -1 | -1 |
| G: -4614.53471 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10879.69892 HOMO: -7.26544 LUMO: -0.05442 factor:1 | 1 (-0.79852) | 1 | 1 |
| G: -4614.53471 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10879.70548 HOMO: -7.09401 LUMO: 0.30749 factor:1 | 1 (-0.80508) | 1 | 1 |
| G: -4614.53471 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10879.64363 HOMO: -6.14705 LUMO: -0.88709 factor:1 | 1 (-0.74322) | -1 | -1 |
| G: -4614.53471 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10879.67965 HOMO: -6.53617 LUMO: -0.28572 factor:1 | 1 (-0.77925) | -1 | -1 |
| G: -4614.53471 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10879.48896 HOMO: -6.37291 LUMO: -0.67212 factor:1 | 1 (-0.58856) | -1 | -1 |
| G: -4614.53471 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10880.41376 HOMO: -6.65591 LUMO: 0.03810 factor:1 | 1 (-1.51336) | -1 | -1 |
| G: -4614.53471 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10880.34465 HOMO: -7.11034 LUMO: 0.75103 factor:1 | 1 (-1.44424) | 1 | 1 |
| G: -4614.53471 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10880.16783 HOMO: -6.85183 LUMO: -0.05987 factor:1 | 1 (-1.26742) | -1 | -1 |
| G: -4614.53471 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10880.00162 HOMO: -6.70761 LUMO: -0.05442 factor:1 | 1 (-1.10122) | -1 | -1 |
| G: -4614.53471 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10879.47170 HOMO: -6.23413 LUMO: 0.06259 factor:1 | 1 (-0.57130) | -1 | -1 |
| G: -4614.53471 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10879.84820 HOMO: -6.55794 LUMO: 0.74015 factor:1 | 1 (-0.94780) | -1 | -1 |
| G: -4614.53471 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10879.32903 HOMO: -7.27905 LUMO: 0.26939 factor:1 | 1 (-0.42863) | 1 | 1 |
| G: -4614.53471 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10878.82810 HOMO: -6.34842 LUMO: -0.86804 factor:1 | -1 (0.07230) | -1 | -1 |
| G: -4614.53471 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10877.93497 HOMO: -6.27222 LUMO: 1.46125 factor:1 | -1 (0.96543) | -1 | -1 |
| G: -4614.53471 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10877.72626 HOMO: -6.65046 LUMO: 2.04902 factor:1 | -1 (1.17414) | -1 | -1 |
| G: -4614.53471 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10878.70157 HOMO: -7.11850 LUMO: -1.14016 factor:1 | -1 (0.19883) | 1 | -1 |
| G: -4614.53471 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10878.62021 HOMO: -6.88720 LUMO: -1.20274 factor:1 | -1 (0.28020) | -1 | -1 |
| G: -4614.53471 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10878.08191 HOMO: -6.69400 LUMO: -0.31565 factor:1 | -1 (0.81849) | -1 | -1 |
| G: -4614.53471 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10878.54897 HOMO: -6.95523 LUMO: -1.55377 factor:1 | -1 (0.35144) | -1 | -1 |
| G: -4614.53471 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10878.63906 HOMO: -6.41372 LUMO: -0.83539 factor:1 | -1 (0.26134) | -1 | -1 |
| G: -4614.53471 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10878.62225 HOMO: -6.13889 LUMO: -0.90070 factor:1 | -1 (0.27815) | -1 | -1 |
| G: -4614.53471 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10878.85460 HOMO: -6.44366 LUMO: -0.55511 factor:1 | -1 (0.04580) | -1 | -1 |
| G: -4614.53471 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10878.42975 HOMO: -6.10079 LUMO: -0.71022 factor:1 | -1 (0.47065) | -1 | -1 |
| G: -4614.53471 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10879.09409 HOMO: -6.90353 LUMO: -0.64763 factor:1 | 1 (-0.19369) | -1 | -1 |
| G: -4614.53471 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10878.75335 HOMO: -6.65046 LUMO: -0.82450 factor:1 | -1 (0.14705) | -1 | -1 |
| G: -4614.53471 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10878.78769 HOMO: -6.81645 LUMO: -0.85444 factor:1 | -1 (0.11271) | -1 | -1 |
| G: -4614.53471 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10876.69859 HOMO: -6.20692 LUMO: 1.30887 factor:1 | -1 (2.20181) | -1 | -1 |
| G: -4614.53471 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10876.70537 HOMO: -5.96201 LUMO: 1.33880 factor:1 | -1 (2.19503) | -1 | -1 |
| G: -4614.53471 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10877.68977 HOMO: -6.52529 LUMO: 1.58914 factor:1 | -1 (1.21063) | -1 | -1 |
| G: -4614.53471 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10877.68865 HOMO: -6.58516 LUMO: 1.97555 factor:1 | -1 (1.21175) | -1 | -1 |
| G: -4614.53471 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10879.73255 HOMO: -6.84366 LUMO: 0.15783 factor:1 | 1 (-0.83215) | -1 | -1 |
| G: -4614.53471 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10879.16220 HOMO: -6.45726 LUMO: 0.42994 factor:1 | 1 (-0.26180) | -1 | -1 |
| G: -4614.53471 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10879.41995 HOMO: -6.75387 LUMO: 0.14422 factor:1 | 1 (-0.51955) | -1 | -1 |
| G: -4614.53471 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10877.76452 HOMO: -6.69944 LUMO: 1.79051 factor:1 | -1 (1.13588) | -1 | -1 |
| G: -4614.53471 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10877.65371 HOMO: -6.59876 LUMO: 1.90208 factor:1 | -1 (1.24669) | -1 | -1 |
| G: -4614.53471 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10878.11484 HOMO: -7.05863 LUMO: 1.20819 factor:1 | -1 (0.78557) | -1 | -1 |
| G: -4614.53471 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10878.83180 HOMO: -6.54978 LUMO: 2.01636 factor:1 | -1 (0.06860) | -1 | -1 |
| G: -4614.53471 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10878.96546 HOMO: -5.52119 LUMO: 1.95106 factor:1 | 1 (-0.06506) | -1 | -1 |
| G: -4614.53471 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10878.39949 HOMO: -6.53617 LUMO: 1.60275 factor:1 | -1 (0.50091) | -1 | -1 |
| G: -4614.53471 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10878.22074 HOMO: -6.11440 LUMO: 1.89119 factor:1 | -1 (0.67966) | -1 | -1 |
| G: -4614.53471 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10879.09221 HOMO: -7.31986 LUMO: 0.48708 factor:1 | 1 (-0.19181) | 1 | 1 |
| G: -4614.53471 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10878.85915 HOMO: -6.76475 LUMO: -0.75648 factor:1 | -1 (0.04125) | -1 | -1 |
| G: -4614.53471 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10878.84269 HOMO: -6.76747 LUMO: -1.06941 factor:1 | -1 (0.05772) | -1 | -1 |
| G: -4614.53471 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10879.76619 HOMO: -6.87087 LUMO: 0.72927 factor:1 | 1 (-0.86578) | -1 | -1 |
| G: -4614.53471 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10879.68654 HOMO: -7.00965 LUMO: 0.02177 factor:1 | 1 (-0.78614) | -1 | -1 |
| G: -4614.53471 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10879.49992 HOMO: -6.54706 LUMO: -0.03265 factor:1 | 1 (-0.59952) | -1 | -1 |
| G: -4614.53471 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10878.59520 HOMO: -6.62325 LUMO: -0.63675 factor:1 | -1 (0.30520) | -1 | -1 |
| G: -4614.53471 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10878.58559 HOMO: -7.03414 LUMO: -1.24084 factor:1 | -1 (0.31481) | -1 | -1 |
| G: -4614.53471 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10878.91292 HOMO: -7.04503 LUMO: -0.10068 factor:1 | 1 (-0.01252) | -1 | -1 |
| G: -4614.53471 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10879.61282 HOMO: -6.67223 LUMO: 0.03537 factor:1 | 1 (-0.71242) | -1 | -1 |
| G: -4614.53471 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10879.52049 HOMO: -6.82734 LUMO: 0.58777 factor:1 | 1 (-0.62009) | -1 | -1 |
| G: -4614.53471 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10879.50185 HOMO: -6.84366 LUMO: 0.46531 factor:1 | 1 (-0.60145) | -1 | -1 |
| G: -4614.53471 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10878.88116 HOMO: -7.03959 LUMO: -1.15104 factor:1 | -1 (0.01924) | -1 | -1 |
| G: -4614.53471 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10879.00233 HOMO: -6.91169 LUMO: -0.41361 factor:1 | 1 (-0.10193) | -1 | -1 |
| G: -4614.53471 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10879.82262 HOMO: -7.10217 LUMO: -0.44627 factor:1 | 1 (-0.92222) | 1 | 1 |
| G: -4614.53471 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10879.70488 HOMO: -6.88176 LUMO: -0.19592 factor:1 | 1 (-0.80448) | -1 | -1 |
| G: -4614.53471 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10879.81258 HOMO: -7.21374 LUMO: -0.46531 factor:1 | 1 (-0.91218) | 1 | 1 |
| G: -4614.53471 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10880.41278 HOMO: -6.54978 LUMO: 0.16871 factor:1 | 1 (-1.51238) | -1 | -1 |
| G: -4614.53471 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10879.84374 HOMO: -6.71305 LUMO: -0.13061 factor:1 | 1 (-0.94334) | -1 | -1 |
| G: -4614.53471 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10879.81955 HOMO: -6.74842 LUMO: -0.36191 factor:1 | 1 (-0.91915) | -1 | -1 |
| G: -4614.53471 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10879.92649 HOMO: -6.74570 LUMO: -0.09796 factor:1 | 1 (-1.02609) | -1 | -1 |
| G: -4614.53471 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10879.83076 HOMO: -6.93890 LUMO: -0.27211 factor:1 | 1 (-0.93036) | -1 | -1 |
| G: -4614.53471 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10879.93650 HOMO: -6.88720 LUMO: -0.18776 factor:1 | 1 (-1.03610) | -1 | -1 |
| G: -4614.53471 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10879.80586 HOMO: -6.74842 LUMO: 0.02993 factor:1 | 1 (-0.90546) | -1 | -1 |
| G: -4614.53471 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10880.21251 HOMO: -6.70216 LUMO: 0.01361 factor:1 | 1 (-1.31211) | -1 | -1 |
| G: -4614.53471 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10880.06295 HOMO: -6.90625 LUMO: 0.00544 factor:1 | 1 (-1.16255) | -1 | -1 |
| G: -4614.53471 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10879.78224 HOMO: -6.18243 LUMO: 0.25851 factor:1 | 1 (-0.88184) | -1 | -1 |
| G: -4614.53471 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10879.45432 HOMO: -6.32937 LUMO: -0.20953 factor:1 | 1 (-0.55391) | -1 | -1 |
| G: -4614.53471 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10879.77035 HOMO: -6.78108 LUMO: 0.00544 factor:1 | 1 (-0.86995) | -1 | -1 |
| G: -4614.53471 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10879.78047 HOMO: -5.97562 LUMO: 0.28572 factor:1 | 1 (-0.88007) | -1 | -1 |
| G: -4614.53471 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10879.57704 HOMO: -5.97290 LUMO: -0.18504 factor:1 | 1 (-0.67664) | -1 | -1 |
| G: -4614.53471 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10879.89430 HOMO: -6.12800 LUMO: 0.42178 factor:1 | 1 (-0.99390) | -1 | -1 |
| G: -4614.53471 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10879.57731 HOMO: -6.24229 LUMO: -0.00816 factor:1 | 1 (-0.67691) | -1 | -1 |
| G: -4614.53471 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10879.93990 HOMO: -6.61781 LUMO: 0.12789 factor:1 | 1 (-1.03950) | -1 | -1 |
| G: -4614.53471 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10879.79691 HOMO: -6.70489 LUMO: 0.14694 factor:1 | 1 (-0.89651) | -1 | -1 |
| G: -4614.53471 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10879.45004 HOMO: -6.86543 LUMO: -0.21225 factor:1 | 1 (-0.54964) | -1 | -1 |
| G: -4614.53471 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10879.35129 HOMO: -6.90081 LUMO: -0.20136 factor:1 | 1 (-0.45089) | -1 | -1 |
| G: -4614.53471 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10879.40923 HOMO: -7.12938 LUMO: -0.25851 factor:1 | 1 (-0.50883) | 1 | 1 |
| G: -4614.53471 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10879.75027 HOMO: -6.93074 LUMO: -0.26667 factor:1 | 1 (-0.84987) | -1 | -1 |
| G: -4614.53471 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10879.61024 HOMO: -7.00421 LUMO: -0.31021 factor:1 | 1 (-0.70984) | -1 | -1 |
| G: -4614.53471 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10879.70186 HOMO: -7.10761 LUMO: -0.17415 factor:1 | 1 (-0.80146) | 1 | 1 |
| G: -5052.27415 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -5658.42769 HOMO: -8.21240 LUMO: 0.05987 factor:2 | 1 (-0.21554) | 1 | 1 |
| G: -5052.27415 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11316.33170 HOMO: -7.14843 LUMO: -0.46531 factor:1 | -1 (0.30814) | 1 | -1 |
| G: -5052.27415 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11317.09585 HOMO: -6.80829 LUMO: -0.29933 factor:1 | 1 (-0.45601) | -1 | -1 |
| G: -5052.27415 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11315.79548 HOMO: -6.84094 LUMO: -0.53606 factor:1 | -1 (0.84437) | -1 | -1 |
| G: -5052.27415 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11315.92666 HOMO: -6.81917 LUMO: -0.26667 factor:1 | -1 (0.71318) | -1 | -1 |
| G: -5052.27415 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11316.09676 HOMO: -6.85727 LUMO: -1.20002 factor:1 | -1 (0.54308) | -1 | -1 |
| G: -5052.27415 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11316.81797 HOMO: -6.39468 LUMO: -1.06941 factor:1 | 1 (-0.17813) | -1 | -1 |
| G: -5052.27415 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11315.87442 HOMO: -6.00827 LUMO: -1.94017 factor:1 | -1 (0.76543) | -1 | -1 |
| G: -5052.27415 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11313.16272 HOMO: -6.80829 LUMO: 0.18504 factor:1 | -1 (3.47713) | -1 | -1 |
| G: -5052.27415 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11315.02583 HOMO: -6.54434 LUMO: -0.95784 factor:1 | -1 (1.61402) | -1 | -1 |
| G: -5052.27415 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11314.04943 HOMO: -6.45454 LUMO: -0.07347 factor:1 | -1 (2.59042) | -1 | -1 |
| G: -5052.27415 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11318.52527 HOMO: -5.33887 LUMO: 1.11839 factor:1 | 1 (-1.88542) | -1 | -1 |
| G: -5052.27415 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11317.62337 HOMO: -5.75249 LUMO: 0.70477 factor:1 | 1 (-0.98353) | -1 | -1 |
| G: -5052.27415 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11318.62086 HOMO: -5.64092 LUMO: 0.87076 factor:1 | 1 (-1.98102) | -1 | -1 |
| G: -5052.27415 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11317.60223 HOMO: -5.14295 LUMO: 1.06124 factor:1 | 1 (-0.96239) | -1 | -1 |
| G: -5052.27415 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11318.57849 HOMO: -5.05043 LUMO: 1.21091 factor:1 | 1 (-1.93865) | -1 | -1 |
| G: -5052.27415 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11318.11103 HOMO: -5.05588 LUMO: 1.02859 factor:1 | 1 (-1.47118) | -1 | -1 |
| G: -5052.27415 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11317.99563 HOMO: -5.76337 LUMO: 0.79457 factor:1 | 1 (-1.35578) | -1 | -1 |
| G: -5052.27415 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11318.17693 HOMO: -5.01506 LUMO: 1.00138 factor:1 | 1 (-1.53709) | -1 | -1 |
| G: -5052.27415 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11318.32616 HOMO: -4.84363 LUMO: 1.53744 factor:1 | 1 (-1.68632) | -1 | -1 |
| G: -5052.27415 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11318.12254 HOMO: -5.17833 LUMO: 1.45309 factor:1 | 1 (-1.48269) | -1 | -1 |
| G: -5052.27415 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11317.87342 HOMO: -5.13751 LUMO: 0.51157 factor:1 | 1 (-1.23357) | -1 | -1 |
| G: -5052.27415 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11317.96605 HOMO: -5.56473 LUMO: 0.32109 factor:1 | 1 (-1.32620) | -1 | -1 |
| G: -5052.27415 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11318.04746 HOMO: -4.69941 LUMO: 1.14016 factor:1 | 1 (-1.40762) | -1 | -1 |
| G: -5052.27415 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11317.41034 HOMO: -4.49260 LUMO: 1.86398 factor:1 | 1 (-0.77049) | -1 | -1 |
| G: -5052.27415 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11317.33480 HOMO: -4.32117 LUMO: 1.68438 factor:1 | 1 (-0.69495) | -1 | -1 |
| G: -5052.27415 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11317.27246 HOMO: -4.44906 LUMO: 1.37690 factor:1 | 1 (-0.63261) | -1 | -1 |
| G: -5052.27415 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11317.27948 HOMO: -4.62049 LUMO: 1.34968 factor:1 | 1 (-0.63963) | -1 | -1 |
| G: -5052.27415 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11317.35267 HOMO: -4.59600 LUMO: 1.58370 factor:1 | 1 (-0.71283) | -1 | -1 |
| G: -5052.27415 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11318.08403 HOMO: -4.98785 LUMO: 1.46669 factor:1 | 1 (-1.44419) | -1 | -1 |
| G: -5052.27415 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11318.31990 HOMO: -5.06676 LUMO: 1.27349 factor:1 | 1 (-1.68006) | -1 | -1 |
| G: -5052.27415 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11318.31803 HOMO: -5.09125 LUMO: 1.13471 factor:1 | 1 (-1.67818) | -1 | -1 |
| G: -5052.27415 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11317.44280 HOMO: -4.84635 LUMO: 1.33608 factor:1 | 1 (-0.80295) | -1 | -1 |
| G: -5052.27415 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11317.19738 HOMO: -4.94431 LUMO: 1.18370 factor:1 | 1 (-0.55753) | -1 | -1 |
| G: -5052.27415 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11317.26859 HOMO: -4.92526 LUMO: 1.39867 factor:1 | 1 (-0.62875) | -1 | -1 |
| G: -5052.27415 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11317.15855 HOMO: -5.71983 LUMO: 0.60137 factor:1 | 1 (-0.51870) | -1 | -1 |
| G: -5052.27415 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11317.75102 HOMO: -5.10486 LUMO: 1.05580 factor:1 | 1 (-1.11118) | -1 | -1 |
| G: -5052.27415 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11317.49670 HOMO: -5.20282 LUMO: 1.01226 factor:1 | 1 (-0.85686) | -1 | -1 |
| G: -5052.27415 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11317.84196 HOMO: -4.98513 LUMO: 1.53744 factor:1 | 1 (-1.20212) | -1 | -1 |
| G: -5052.27415 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11317.61102 HOMO: -5.67085 LUMO: 0.17687 factor:1 | 1 (-0.97117) | -1 | -1 |
| G: -5052.27415 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11317.54329 HOMO: -5.87222 LUMO: 0.12517 factor:1 | 1 (-0.90345) | -1 | -1 |
| G: -5052.27415 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11317.87483 HOMO: -5.20826 LUMO: 0.91702 factor:1 | 1 (-1.23499) | -1 | -1 |
| G: -5052.27415 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11317.62707 HOMO: -5.94569 LUMO: 0.63130 factor:1 | 1 (-0.98723) | -1 | -1 |
| G: -5052.27415 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11317.49534 HOMO: -5.35792 LUMO: 0.91430 factor:1 | 1 (-0.85550) | -1 | -1 |
| G: -5052.27415 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11317.61203 HOMO: -5.36336 LUMO: 1.44220 factor:1 | 1 (-0.97218) | -1 | -1 |
| G: -5052.27415 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11317.56013 HOMO: -5.83412 LUMO: 0.71294 factor:1 | 1 (-0.92029) | -1 | -1 |
| G: -5052.27415 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11317.63692 HOMO: -4.97696 LUMO: 1.72792 factor:1 | 1 (-0.99708) | -1 | -1 |
| G: -5052.27415 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11317.56637 HOMO: -5.55929 LUMO: 0.23130 factor:1 | 1 (-0.92652) | -1 | -1 |
| G: -5052.27415 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11317.72316 HOMO: -5.71167 LUMO: 0.47348 factor:1 | 1 (-1.08331) | -1 | -1 |
| G: -5052.27415 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11317.94063 HOMO: -7.31986 LUMO: -2.54699 factor:1 | 1 (-1.30079) | -1 | -1 |
| G: -5052.27415 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11317.79369 HOMO: -5.34704 LUMO: 1.19730 factor:1 | 1 (-1.15384) | -1 | -1 |
| G: -5052.27415 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11317.70348 HOMO: -5.45860 LUMO: 0.80818 factor:1 | 1 (-1.06364) | -1 | -1 |
| G: -5052.27415 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11318.14766 HOMO: -5.12663 LUMO: 1.20274 factor:1 | 1 (-1.50781) | -1 | -1 |
| G: -5052.27415 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11317.09828 HOMO: -5.37153 LUMO: 1.05580 factor:1 | 1 (-0.45843) | -1 | -1 |
| G: -5052.27415 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11318.04338 HOMO: -5.47221 LUMO: 0.97961 factor:1 | 1 (-1.40354) | -1 | -1 |
| G: -5052.27415 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11317.16549 HOMO: -5.06948 LUMO: 1.12111 factor:1 | 1 (-0.52564) | -1 | -1 |
| G: -5052.27415 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11318.07497 HOMO: -5.19737 LUMO: 1.25444 factor:1 | 1 (-1.43513) | -1 | -1 |
| G: -5052.27415 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11317.03539 HOMO: -5.27901 LUMO: 1.00682 factor:1 | 1 (-0.39554) | -1 | -1 |
| G: -5052.27415 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11317.39042 HOMO: -5.38513 LUMO: 0.49253 factor:1 | 1 (-0.75057) | -1 | -1 |
| G: -5052.27415 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11318.33590 HOMO: -5.12390 LUMO: 1.22995 factor:1 | 1 (-1.69606) | -1 | -1 |
| G: -5052.27415 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11317.30661 HOMO: -5.31438 LUMO: 0.70205 factor:1 | 1 (-0.66676) | -1 | -1 |
| G: -5052.27415 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11317.64335 HOMO: -5.17561 LUMO: 1.04492 factor:1 | 1 (-1.00350) | -1 | -1 |
| G: -5052.27415 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11317.80359 HOMO: -4.94431 LUMO: 1.52656 factor:1 | 1 (-1.16375) | -1 | -1 |
| G: -5052.27415 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11317.59393 HOMO: -5.13751 LUMO: 0.93879 factor:1 | 1 (-0.95409) | -1 | -1 |
| G: -5052.27415 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11317.69004 HOMO: -5.49942 LUMO: 0.97689 factor:1 | 1 (-1.05020) | -1 | -1 |
| G: -5052.27415 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11318.20872 HOMO: -5.79058 LUMO: 0.53879 factor:1 | 1 (-1.56887) | -1 | -1 |
| G: -5052.27415 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11317.90615 HOMO: -5.36881 LUMO: 1.56465 factor:1 | 1 (-1.26631) | -1 | -1 |
| G: -5052.27415 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11317.27409 HOMO: -4.67492 LUMO: 1.32792 factor:1 | 1 (-0.63424) | -1 | -1 |
| G: -5052.27415 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11317.34179 HOMO: -4.60145 LUMO: 1.19458 factor:1 | 1 (-0.70194) | -1 | -1 |
| G: -5052.27415 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11317.31346 HOMO: -4.49260 LUMO: 1.60547 factor:1 | 1 (-0.67362) | -1 | -1 |
| G: -5052.27415 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11317.14304 HOMO: -4.65043 LUMO: 1.34696 factor:1 | 1 (-0.50319) | -1 | -1 |
| G: -5052.27415 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11317.20331 HOMO: -4.77560 LUMO: 1.35241 factor:1 | 1 (-0.56347) | -1 | -1 |
| G: -5052.27415 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11317.36606 HOMO: -4.94431 LUMO: 1.17825 factor:1 | 1 (-0.72622) | -1 | -1 |
| G: -5052.27415 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11318.38916 HOMO: -4.87084 LUMO: 1.41771 factor:1 | 1 (-1.74931) | -1 | -1 |
| G: -5052.27415 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11318.23819 HOMO: -5.34432 LUMO: 1.16737 factor:1 | 1 (-1.59834) | -1 | -1 |
| G: -5052.27415 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11317.90675 HOMO: -4.94975 LUMO: 1.67622 factor:1 | 1 (-1.26691) | -1 | -1 |
| G: -5052.27415 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11317.75532 HOMO: -4.81369 LUMO: 1.14288 factor:1 | 1 (-1.11548) | -1 | -1 |
| G: -5052.27415 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11317.42174 HOMO: -5.22459 LUMO: 0.29660 factor:1 | 1 (-0.78189) | -1 | -1 |
| G: -5052.27415 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11317.24769 HOMO: -5.21642 LUMO: 0.37824 factor:1 | 1 (-0.60785) | -1 | -1 |
| G: -5052.27415 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11317.46615 HOMO: -5.00417 LUMO: 1.01226 factor:1 | 1 (-0.82630) | -1 | -1 |
| G: -5052.27415 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11317.54623 HOMO: -5.46677 LUMO: 0.10612 factor:1 | 1 (-0.90638) | -1 | -1 |
| G: -5052.27415 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11317.85549 HOMO: -5.51303 LUMO: 0.54151 factor:1 | 1 (-1.21564) | -1 | -1 |
| G: -5052.27415 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11317.29624 HOMO: -5.63004 LUMO: 0.17960 factor:1 | 1 (-0.65639) | -1 | -1 |
| G: -5052.27415 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11317.47910 HOMO: -4.79193 LUMO: 1.12111 factor:1 | 1 (-0.83925) | -1 | -1 |
| G: -5052.27415 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11317.55652 HOMO: -5.43411 LUMO: 0.45987 factor:1 | 1 (-0.91667) | -1 | -1 |
| G: -5052.27415 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11317.97345 HOMO: -7.06135 LUMO: -2.13881 factor:1 | 1 (-1.33360) | 1 | 1 |
| G: -5052.27415 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11317.76607 HOMO: -5.33071 LUMO: 1.14016 factor:1 | 1 (-1.12622) | -1 | -1 |
| G: -5052.27415 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11318.14463 HOMO: -7.12394 LUMO: -0.03810 factor:1 | 1 (-1.50479) | 1 | 1 |
| G: -5052.27415 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11318.28725 HOMO: -7.20558 LUMO: -2.50889 factor:1 | 1 (-1.64740) | 1 | 1 |
| G: -5052.27415 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11318.27947 HOMO: -7.26816 LUMO: -2.11432 factor:1 | 1 (-1.63962) | 1 | 1 |
| G: -5052.27415 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11318.62225 HOMO: -7.89674 LUMO: 0.31021 factor:1 | 1 (-1.98240) | 1 | 1 |
| G: -5052.27415 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11318.09070 HOMO: -7.26544 LUMO: 0.22858 factor:1 | 1 (-1.45086) | 1 | 1 |
| G: -5052.27415 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11317.56783 HOMO: -7.12666 LUMO: -0.02449 factor:1 | 1 (-0.92799) | 1 | 1 |
| G: -5052.27415 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11318.65490 HOMO: -7.68722 LUMO: 0.71838 factor:1 | 1 (-2.01506) | 1 | 1 |
| G: -5052.27415 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11318.01470 HOMO: -6.86271 LUMO: -0.96056 factor:1 | 1 (-1.37486) | -1 | -1 |
| G: -5052.27415 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11318.20717 HOMO: -7.07496 LUMO: -1.11839 factor:1 | 1 (-1.56732) | 1 | 1 |
| G: -5052.27415 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11318.53006 HOMO: -7.06952 LUMO: -2.08439 factor:1 | 1 (-1.89021) | 1 | 1 |
| G: -5052.27415 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11318.26739 HOMO: -6.60965 LUMO: -2.11977 factor:1 | 1 (-1.62754) | -1 | -1 |
| G: -5052.27415 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11317.86376 HOMO: -6.87360 LUMO: -1.85854 factor:1 | 1 (-1.22391) | -1 | -1 |
| G: -5052.27415 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11318.25704 HOMO: -7.67089 LUMO: -0.24762 factor:1 | 1 (-1.61720) | 1 | 1 |
| G: -5052.27415 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11317.89984 HOMO: -6.45726 LUMO: -1.86398 factor:1 | 1 (-1.26000) | -1 | -1 |
| G: -5052.27415 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11317.87353 HOMO: -6.91713 LUMO: 0.33198 factor:1 | 1 (-1.23368) | -1 | -1 |
| G: -5052.27415 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11318.44709 HOMO: -6.83278 LUMO: 0.26667 factor:1 | 1 (-1.80724) | -1 | -1 |
| G: -5052.27415 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11317.90436 HOMO: -6.89264 LUMO: -1.00682 factor:1 | 1 (-1.26451) | -1 | -1 |
| G: -5052.27415 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11317.73453 HOMO: -6.57427 LUMO: 0.22041 factor:1 | 1 (-1.09469) | -1 | -1 |
| G: -5052.27415 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11317.53518 HOMO: -7.52123 LUMO: -0.01905 factor:1 | 1 (-0.89534) | 1 | 1 |
| G: -5052.27415 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11318.62715 HOMO: -7.37429 LUMO: -0.08980 factor:1 | 1 (-1.98730) | 1 | 1 |
| G: -5052.27415 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11318.64832 HOMO: -7.28449 LUMO: -0.26395 factor:1 | 1 (-2.00847) | 1 | 1 |
| G: -5052.27415 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11317.89807 HOMO: -6.79740 LUMO: -0.60954 factor:1 | 1 (-1.25823) | -1 | -1 |
| G: -5052.27415 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11318.03386 HOMO: -7.12666 LUMO: -0.60681 factor:1 | 1 (-1.39401) | 1 | 1 |
| G: -5052.27415 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11318.59623 HOMO: -6.96611 LUMO: -0.30477 factor:1 | 1 (-1.95639) | -1 | -1 |
| G: -5052.27415 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11319.47688 HOMO: -7.08040 LUMO: -0.31293 factor:1 | 1 (-2.83703) | 1 | 1 |
| G: -5052.27415 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11318.71999 HOMO: -6.78924 LUMO: -0.73743 factor:1 | 1 (-2.08015) | -1 | -1 |
| G: -5052.27415 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11317.74158 HOMO: -7.57293 LUMO: -1.11295 factor:1 | 1 (-1.10173) | 1 | 1 |
| G: -5052.27415 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11319.58515 HOMO: -7.15932 LUMO: -0.23130 factor:1 | 1 (-2.94531) | 1 | 1 |
| G: -5052.27415 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11318.86323 HOMO: -7.48585 LUMO: -0.10068 factor:1 | 1 (-2.22339) | 1 | 1 |
| G: -5052.27415 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11318.81624 HOMO: -7.17020 LUMO: -0.26123 factor:1 | 1 (-2.17639) | 1 | 1 |
| G: -5052.27415 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11318.89434 HOMO: -7.43143 LUMO: -0.16055 factor:1 | 1 (-2.25449) | 1 | 1 |
| G: -5052.27415 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11318.68935 HOMO: -7.14843 LUMO: -0.10612 factor:1 | 1 (-2.04951) | 1 | 1 |
| G: -5052.27415 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11319.41764 HOMO: -6.95523 LUMO: -0.22585 factor:1 | 1 (-2.77779) | -1 | -1 |
| G: -5052.27415 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11318.27451 HOMO: -7.06680 LUMO: -0.51974 factor:1 | 1 (-1.63467) | 1 | 1 |
| G: -5052.27415 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11319.04307 HOMO: -6.80829 LUMO: -0.64763 factor:1 | 1 (-2.40323) | -1 | -1 |
| G: -5052.27415 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11318.29204 HOMO: -7.13210 LUMO: -0.48164 factor:1 | 1 (-1.65219) | 1 | 1 |
| G: -5052.27415 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11318.40807 HOMO: -7.16204 LUMO: -0.45715 factor:1 | 1 (-1.76822) | 1 | 1 |
| G: -5052.27415 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11318.45871 HOMO: -7.15115 LUMO: -0.43266 factor:1 | 1 (-1.81886) | 1 | 1 |
| G: -5052.27415 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11317.77410 HOMO: -7.15932 LUMO: -2.52794 factor:1 | 1 (-1.13425) | -1 | -1 |
| G: -5052.27415 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11317.69412 HOMO: -7.21102 LUMO: -2.65311 factor:1 | 1 (-1.05428) | -1 | -1 |
| G: -5052.27415 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11317.42193 HOMO: -6.57427 LUMO: -2.78645 factor:1 | 1 (-0.78208) | -1 | -1 |
| G: -5052.27415 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11317.46808 HOMO: -6.40828 LUMO: -3.23815 factor:1 | 1 (-0.82823) | -1 | -1 |
| G: -5052.27415 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11318.02439 HOMO: -7.71987 LUMO: -0.20953 factor:1 | 1 (-1.38454) | 1 | 1 |
| G: -5052.27415 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11317.84038 HOMO: -7.47769 LUMO: -0.43810 factor:1 | 1 (-1.20054) | 1 | 1 |
| G: -5052.27415 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11317.31482 HOMO: -6.68040 LUMO: -2.22589 factor:1 | 1 (-0.67498) | -1 | -1 |
| G: -5052.27415 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11317.58087 HOMO: -6.92802 LUMO: -1.99187 factor:1 | 1 (-0.94102) | -1 | -1 |
| G: -5052.27415 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11317.54914 HOMO: -7.73620 LUMO: 0.01633 factor:1 | 1 (-0.90930) | 1 | 1 |
| G: -5052.27415 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11317.76479 HOMO: -7.28721 LUMO: -0.18504 factor:1 | 1 (-1.12495) | 1 | 1 |
| G: -5052.27415 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11316.79748 HOMO: -7.49674 LUMO: -0.19864 factor:1 | 1 (-0.15764) | 1 | 1 |
| G: -5052.27415 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11318.02450 HOMO: -7.10489 LUMO: -2.56331 factor:1 | 1 (-1.38465) | -1 | -1 |
| G: -5052.27415 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11318.36396 HOMO: -7.36612 LUMO: 0.16055 factor:1 | 1 (-1.72411) | 1 | 1 |
| G: -5052.27415 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11318.34945 HOMO: -7.67633 LUMO: 0.33198 factor:1 | 1 (-1.70961) | 1 | 1 |
| G: -5052.27415 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11317.84259 HOMO: -7.07768 LUMO: -0.27483 factor:1 | 1 (-1.20274) | 1 | 1 |
| G: -5052.27415 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11317.71758 HOMO: -7.32531 LUMO: 0.05442 factor:1 | 1 (-1.07773) | 1 | 1 |
| G: -5052.27415 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11316.73732 HOMO: -6.79740 LUMO: -1.21635 factor:1 | 1 (-0.09747) | -1 | -1 |
| G: -5052.27415 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11316.38615 HOMO: -7.14027 LUMO: 0.12517 factor:1 | -1 (0.25369) | 1 | -1 |
| G: -5052.27415 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11316.32953 HOMO: -7.17292 LUMO: 0.16871 factor:1 | -1 (0.31032) | 1 | -1 |
| G: -5052.27415 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11317.74090 HOMO: -7.08312 LUMO: -1.38778 factor:1 | 1 (-1.10105) | 1 | 1 |
| G: -5052.27415 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11317.69546 HOMO: -6.75387 LUMO: -1.88031 factor:1 | 1 (-1.05561) | -1 | -1 |
| G: -5052.27415 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11317.89494 HOMO: -7.07768 LUMO: -1.25717 factor:1 | 1 (-1.25510) | 1 | 1 |
| G: -5052.27415 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11317.33390 HOMO: -6.46543 LUMO: -1.14016 factor:1 | 1 (-0.69405) | -1 | -1 |
| G: -5052.27415 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11317.47338 HOMO: -7.37973 LUMO: -0.45987 factor:1 | 1 (-0.83354) | 1 | 1 |
| G: -5052.27415 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11317.77608 HOMO: -7.46408 LUMO: 0.03265 factor:1 | 1 (-1.13624) | 1 | 1 |
| G: -5052.27415 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11316.80007 HOMO: -7.96477 LUMO: -0.19864 factor:1 | 1 (-0.16022) | 1 | 1 |
| G: -5052.27415 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11318.02907 HOMO: -6.93890 LUMO: -1.11839 factor:1 | 1 (-1.38922) | -1 | -1 |
| G: -5052.27415 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11318.14942 HOMO: -7.06408 LUMO: -1.08846 factor:1 | 1 (-1.50958) | 1 | 1 |
| G: -5052.27415 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11317.68084 HOMO: -7.14027 LUMO: -0.33470 factor:1 | 1 (-1.04100) | 1 | 1 |
| G: -5052.27415 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11318.13508 HOMO: -7.38245 LUMO: 0.10885 factor:1 | 1 (-1.49524) | 1 | 1 |
| G: -5052.27415 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11318.94963 HOMO: -7.59470 LUMO: -1.21363 factor:1 | 1 (-2.30978) | 1 | 1 |
| G: -5052.27415 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11317.58530 HOMO: -7.23279 LUMO: -1.23812 factor:1 | 1 (-0.94546) | 1 | 1 |
| G: -5052.27415 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11318.06950 HOMO: -6.90897 LUMO: 0.23402 factor:1 | 1 (-1.42966) | -1 | -1 |
| G: -5052.27415 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11317.17270 HOMO: -7.36340 LUMO: -0.17143 factor:1 | 1 (-0.53285) | 1 | 1 |
| G: -5052.27415 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11317.96746 HOMO: -6.61781 LUMO: -0.01361 factor:1 | 1 (-1.32762) | -1 | -1 |
| G: -5052.27415 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11318.90702 HOMO: -6.80013 LUMO: 0.38368 factor:1 | 1 (-2.26717) | -1 | -1 |
| G: -5052.27415 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11318.63365 HOMO: -6.72121 LUMO: -0.95512 factor:1 | 1 (-1.99381) | -1 | -1 |
| G: -5052.27415 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11317.83415 HOMO: -6.24773 LUMO: -0.69933 factor:1 | 1 (-1.19431) | -1 | -1 |
| G: -5052.27415 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11318.11691 HOMO: -6.56883 LUMO: 0.14694 factor:1 | 1 (-1.47706) | -1 | -1 |
| G: -5052.27415 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11317.59091 HOMO: -6.51441 LUMO: -1.27621 factor:1 | 1 (-0.95107) | -1 | -1 |
| G: -5052.27415 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11318.42295 HOMO: -6.91986 LUMO: -1.16737 factor:1 | 1 (-1.78311) | -1 | -1 |
| G: -5052.27415 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11317.78817 HOMO: -6.17971 LUMO: -0.65307 factor:1 | 1 (-1.14832) | -1 | -1 |
| G: -5052.27415 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11318.62892 HOMO: -7.22462 LUMO: 0.04354 factor:1 | 1 (-1.98907) | 1 | 1 |
| G: -5052.27415 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11318.57719 HOMO: -7.16204 LUMO: -0.23674 factor:1 | 1 (-1.93734) | 1 | 1 |
| G: -5052.27415 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11318.45332 HOMO: -6.81645 LUMO: -0.19320 factor:1 | 1 (-1.81348) | -1 | -1 |
| G: -5052.27415 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11318.42124 HOMO: -6.69400 LUMO: 0.04082 factor:1 | 1 (-1.78139) | -1 | -1 |
| G: -5052.27415 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11318.02795 HOMO: -6.63141 LUMO: -0.22858 factor:1 | 1 (-1.38811) | -1 | -1 |
| G: -5052.27415 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11316.63247 HOMO: -6.92258 LUMO: -1.11295 factor:1 | -1 (0.00737) | -1 | -1 |
| G: -5052.27415 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11317.73782 HOMO: -6.60148 LUMO: -1.13744 factor:1 | 1 (-1.09798) | -1 | -1 |
| G: -5052.27415 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11317.16462 HOMO: -6.78108 LUMO: -0.82450 factor:1 | 1 (-0.52477) | -1 | -1 |
| G: -5052.27415 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11317.23270 HOMO: -7.05591 LUMO: -0.97145 factor:1 | 1 (-0.59285) | -1 | -1 |
| G: -5052.27415 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11318.03288 HOMO: -6.65318 LUMO: -1.26261 factor:1 | 1 (-1.39303) | -1 | -1 |
| G: -5052.27415 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11317.90596 HOMO: -6.98244 LUMO: -0.98233 factor:1 | 1 (-1.26612) | -1 | -1 |
| G: -5052.27415 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11317.12013 HOMO: -7.11850 LUMO: -0.99594 factor:1 | 1 (-0.48028) | 1 | 1 |
| G: -5052.27415 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11318.66813 HOMO: -6.64230 LUMO: -0.93879 factor:1 | 1 (-2.02828) | -1 | -1 |
| G: -5052.27415 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11318.22543 HOMO: -6.62053 LUMO: -1.22451 factor:1 | 1 (-1.58558) | -1 | -1 |
| G: -5052.27415 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11317.88858 HOMO: -7.02598 LUMO: -0.85172 factor:1 | 1 (-1.24873) | -1 | -1 |
| G: -5052.27415 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11318.14572 HOMO: -7.06680 LUMO: -0.89253 factor:1 | 1 (-1.50588) | 1 | 1 |
| G: -5052.27415 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11317.04832 HOMO: -7.17292 LUMO: 0.00272 factor:1 | 1 (-0.40847) | 1 | 1 |
| G: -5052.27415 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11318.14142 HOMO: -7.03142 LUMO: -0.35103 factor:1 | 1 (-1.50158) | -1 | -1 |
| G: -5052.27415 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11318.04564 HOMO: -6.96884 LUMO: -0.09796 factor:1 | 1 (-1.40579) | -1 | -1 |
| G: -5052.27415 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11317.72487 HOMO: -6.56339 LUMO: -0.99322 factor:1 | 1 (-1.08503) | -1 | -1 |
| G: -5052.27415 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11318.75425 HOMO: -7.08857 LUMO: -0.17687 factor:1 | 1 (-2.11441) | 1 | 1 |
| G: -5052.27415 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11318.65488 HOMO: -7.05863 LUMO: -0.22041 factor:1 | 1 (-2.01503) | -1 | -1 |
| G: -5052.27415 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11319.48637 HOMO: -7.15115 LUMO: -0.17960 factor:1 | 1 (-2.84653) | 1 | 1 |
| G: -5052.27415 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11317.53804 HOMO: -6.67495 LUMO: -0.96600 factor:1 | 1 (-0.89819) | -1 | -1 |
| G: -5052.27415 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11317.76212 HOMO: -6.74026 LUMO: -1.79867 factor:1 | 1 (-1.12228) | -1 | -1 |
| G: -5052.27415 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11317.44054 HOMO: -6.73482 LUMO: -1.78235 factor:1 | 1 (-0.80070) | -1 | -1 |
| G: -5052.27415 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11316.20797 HOMO: -6.09807 LUMO: 0.16871 factor:1 | -1 (0.43187) | -1 | -1 |
| G: -5052.27415 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11315.62108 HOMO: -6.72393 LUMO: 0.27211 factor:1 | -1 (1.01877) | -1 | -1 |
| G: -5052.27415 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11316.26201 HOMO: -6.40556 LUMO: -0.04354 factor:1 | -1 (0.37783) | -1 | -1 |
| G: -5052.27415 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11315.54831 HOMO: -6.56883 LUMO: 0.22041 factor:1 | -1 (1.09153) | -1 | -1 |
| G: -5052.27415 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11317.44522 HOMO: -7.22462 LUMO: 0.15783 factor:1 | 1 (-0.80538) | 1 | 1 |
| G: -5052.27415 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11317.15055 HOMO: -6.83550 LUMO: 0.19320 factor:1 | 1 (-0.51070) | -1 | -1 |
| G: -5052.27415 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11316.47731 HOMO: -7.26816 LUMO: -0.07619 factor:1 | -1 (0.16253) | 1 | -1 |
| G: -5052.27415 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11318.09655 HOMO: -7.13483 LUMO: 0.33198 factor:1 | 1 (-1.45671) | 1 | 1 |
| G: -5052.27415 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11318.02341 HOMO: -6.58243 LUMO: -0.26395 factor:1 | 1 (-1.38356) | -1 | -1 |
| G: -5052.27415 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11317.22516 HOMO: -7.38517 LUMO: 0.17143 factor:1 | 1 (-0.58532) | 1 | 1 |
| G: -5052.27415 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11318.53204 HOMO: -6.80013 LUMO: 0.25851 factor:1 | 1 (-1.89220) | -1 | -1 |
| G: -5052.27415 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11317.86332 HOMO: -6.96611 LUMO: 0.11429 factor:1 | 1 (-1.22348) | -1 | -1 |
| G: -5052.27415 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11317.50416 HOMO: -6.51713 LUMO: -1.14560 factor:1 | 1 (-0.86432) | -1 | -1 |
| G: -5052.27415 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11318.94089 HOMO: -7.15387 LUMO: -0.35647 factor:1 | 1 (-2.30105) | 1 | 1 |
| G: -5052.27415 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11317.75562 HOMO: -5.26540 LUMO: 1.26805 factor:1 | 1 (-1.11578) | -1 | -1 |
| G: -5052.27415 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11317.61042 HOMO: -6.76475 LUMO: -0.16327 factor:1 | 1 (-0.97058) | -1 | -1 |
| G: -5052.27415 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11317.21738 HOMO: -6.55250 LUMO: -0.71838 factor:1 | 1 (-0.57753) | -1 | -1 |
| G: -5052.27415 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11317.34350 HOMO: -6.76203 LUMO: -1.08301 factor:1 | 1 (-0.70366) | -1 | -1 |
| G: -5052.27415 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11317.20092 HOMO: -7.14027 LUMO: -0.01633 factor:1 | 1 (-0.56107) | 1 | 1 |
| G: -5052.27415 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11318.26752 HOMO: -6.94979 LUMO: -0.93879 factor:1 | 1 (-1.62768) | -1 | -1 |
| G: -5052.27415 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11318.23002 HOMO: -6.74842 LUMO: 0.31293 factor:1 | 1 (-1.59018) | -1 | -1 |
| G: -5052.27415 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11318.25979 HOMO: -6.43821 LUMO: 0.05987 factor:1 | 1 (-1.61995) | -1 | -1 |
| G: -5052.27415 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11318.27427 HOMO: -6.60420 LUMO: 0.22585 factor:1 | 1 (-1.63442) | -1 | -1 |
| G: -5052.27415 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11318.25977 HOMO: -6.43821 LUMO: 0.05987 factor:1 | 1 (-1.61992) | -1 | -1 |
| G: -5052.27415 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11317.40870 HOMO: -6.34570 LUMO: 1.43948 factor:1 | 1 (-0.76886) | -1 | -1 |
| G: -5052.27415 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11316.68194 HOMO: -6.03004 LUMO: 1.21363 factor:1 | 1 (-0.04210) | -1 | -1 |
| G: -5052.27415 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11317.60702 HOMO: -6.68040 LUMO: -0.92247 factor:1 | 1 (-0.96717) | -1 | -1 |
| G: -5052.27415 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11317.90754 HOMO: -6.92530 LUMO: -0.31293 factor:1 | 1 (-1.26770) | -1 | -1 |
| G: -5052.27415 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11318.09038 HOMO: -6.94979 LUMO: -0.19864 factor:1 | 1 (-1.45053) | -1 | -1 |
| G: -5052.27415 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11318.75305 HOMO: -6.80829 LUMO: -0.30477 factor:1 | 1 (-2.11321) | -1 | -1 |
| G: -5052.27415 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11317.34348 HOMO: -7.22734 LUMO: -1.02859 factor:1 | 1 (-0.70363) | 1 | 1 |
| G: -5052.27415 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11318.07555 HOMO: -6.93890 LUMO: -0.72382 factor:1 | 1 (-1.43570) | -1 | -1 |
| G: -5052.27415 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11317.10568 HOMO: -7.27088 LUMO: -0.78097 factor:1 | 1 (-0.46583) | 1 | 1 |
| G: -5052.27415 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11316.91073 HOMO: -7.29809 LUMO: -0.97145 factor:1 | 1 (-0.27089) | 1 | 1 |
| G: -5052.27415 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11317.11996 HOMO: -7.18925 LUMO: -0.94696 factor:1 | 1 (-0.48012) | 1 | 1 |
| G: -5052.27415 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11317.03245 HOMO: -7.33891 LUMO: -0.96873 factor:1 | 1 (-0.39261) | 1 | 1 |
| G: -5052.27415 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11317.09387 HOMO: -7.36068 LUMO: -0.28028 factor:1 | 1 (-0.45402) | 1 | 1 |
| G: -5052.27415 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11317.48789 HOMO: -7.10761 LUMO: -1.14832 factor:1 | 1 (-0.84804) | 1 | 1 |
| G: -5052.27415 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11317.59951 HOMO: -6.94707 LUMO: -0.65307 factor:1 | 1 (-0.95966) | -1 | -1 |
| G: -5052.27415 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11316.79381 HOMO: -6.91713 LUMO: -1.81228 factor:1 | 1 (-0.15396) | -1 | -1 |
| G: -5052.27415 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11317.54756 HOMO: -6.78652 LUMO: -2.01636 factor:1 | 1 (-0.90772) | -1 | -1 |
| G: -5052.27415 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11317.74642 HOMO: -6.52801 LUMO: -1.17553 factor:1 | 1 (-1.10658) | -1 | -1 |
| G: -5052.27415 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11316.32740 HOMO: -7.54844 LUMO: -1.18642 factor:1 | -1 (0.31244) | 1 | -1 |
| G: -5052.27415 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11316.28476 HOMO: -7.52939 LUMO: -1.23812 factor:1 | -1 (0.35508) | 1 | -1 |
| G: -5052.27415 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11316.95152 HOMO: -7.94572 LUMO: -0.81634 factor:1 | 1 (-0.31168) | 1 | 1 |
| G: -5052.27415 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11316.93103 HOMO: -7.55932 LUMO: -0.86260 factor:1 | 1 (-0.29119) | 1 | 1 |
| G: -5052.27415 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11315.81308 HOMO: -7.72259 LUMO: -1.39050 factor:1 | -1 (0.82676) | 1 | -1 |
| G: -5052.27415 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11316.46180 HOMO: -7.11850 LUMO: -1.01498 factor:1 | -1 (0.17804) | 1 | -1 |
| G: -5052.27415 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11316.39785 HOMO: -7.09673 LUMO: -1.00954 factor:1 | -1 (0.24199) | 1 | -1 |
| G: -5052.27415 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11316.92581 HOMO: -6.06270 LUMO: 0.16327 factor:1 | 1 (-0.28596) | -1 | -1 |
| G: -5052.27415 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11317.12228 HOMO: -5.71167 LUMO: 0.70477 factor:1 | 1 (-0.48243) | -1 | -1 |
| G: -5052.27415 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11317.55507 HOMO: -5.38241 LUMO: 0.86260 factor:1 | 1 (-0.91523) | -1 | -1 |
| G: -5052.27415 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11317.66566 HOMO: -5.67357 LUMO: 1.27621 factor:1 | 1 (-1.02581) | -1 | -1 |
| G: -5052.27415 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11317.19036 HOMO: -7.56204 LUMO: -0.68573 factor:1 | 1 (-0.55051) | 1 | 1 |
| G: -5052.27415 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11317.35629 HOMO: -5.57833 LUMO: 1.13199 factor:1 | 1 (-0.71645) | -1 | -1 |
| G: -5052.27415 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11317.18160 HOMO: -7.58653 LUMO: -0.66124 factor:1 | 1 (-0.54175) | 1 | 1 |
| G: -5052.27415 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11315.96990 HOMO: -7.91851 LUMO: -1.10206 factor:1 | -1 (0.66994) | 1 | -1 |
| G: -5052.27415 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11316.54901 HOMO: -6.48992 LUMO: -1.00138 factor:1 | -1 (0.09083) | -1 | -1 |
| G: -5052.27415 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11317.42911 HOMO: -7.09673 LUMO: -0.45171 factor:1 | 1 (-0.78927) | 1 | 1 |
| G: -5052.27415 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11318.38298 HOMO: -6.63686 LUMO: 0.09252 factor:1 | 1 (-1.74313) | -1 | -1 |
| G: -5052.27415 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11316.95871 HOMO: -6.84366 LUMO: -0.14422 factor:1 | 1 (-0.31886) | -1 | -1 |
| G: -5052.27415 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11317.89943 HOMO: -6.93074 LUMO: 0.04354 factor:1 | 1 (-1.25959) | -1 | -1 |
| G: -5052.27415 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11317.63437 HOMO: -6.90353 LUMO: -0.19864 factor:1 | 1 (-0.99452) | -1 | -1 |
| G: -5052.27415 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11318.11936 HOMO: -6.59876 LUMO: -0.10068 factor:1 | 1 (-1.47951) | -1 | -1 |
| G: -5052.27415 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11316.45233 HOMO: -6.74570 LUMO: -0.44627 factor:1 | -1 (0.18751) | -1 | -1 |
| G: -5052.27415 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11316.30566 HOMO: -6.60148 LUMO: -0.61770 factor:1 | -1 (0.33418) | -1 | -1 |
| G: -5052.27415 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11316.09379 HOMO: -6.55794 LUMO: -1.06941 factor:1 | -1 (0.54605) | -1 | -1 |
| G: -5052.27415 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11316.97362 HOMO: -7.12666 LUMO: -0.11973 factor:1 | 1 (-0.33377) | 1 | 1 |
| G: -5052.27415 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11316.92649 HOMO: -7.21646 LUMO: -0.50069 factor:1 | 1 (-0.28664) | 1 | 1 |
| G: -5052.27415 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11315.76236 HOMO: -7.27632 LUMO: -1.00682 factor:1 | -1 (0.87749) | 1 | -1 |
| G: -5052.27415 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11317.90117 HOMO: -6.74298 LUMO: 0.04354 factor:1 | 1 (-1.26133) | -1 | -1 |
| G: -5052.27415 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11318.43147 HOMO: -6.37291 LUMO: 0.14150 factor:1 | 1 (-1.79162) | -1 | -1 |
| G: -5052.27415 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11317.52422 HOMO: -5.61371 LUMO: 1.28438 factor:1 | 1 (-0.88437) | -1 | -1 |
| G: -5052.27415 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11317.15806 HOMO: -5.52119 LUMO: 0.99866 factor:1 | 1 (-0.51821) | -1 | -1 |
| G: -5052.27415 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11316.80964 HOMO: -6.51985 LUMO: -0.10885 factor:1 | 1 (-0.16980) | -1 | -1 |
| G: -5052.27415 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11316.78423 HOMO: -5.61371 LUMO: 0.77280 factor:1 | 1 (-0.14438) | -1 | -1 |
| G: -5052.27415 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11316.42596 HOMO: -5.58922 LUMO: 0.24490 factor:1 | -1 (0.21388) | -1 | -1 |
| G: -5052.27415 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11316.35908 HOMO: -6.32665 LUMO: -0.57144 factor:1 | -1 (0.28077) | -1 | -1 |
| G: -5052.27415 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11316.26408 HOMO: -6.29127 LUMO: -0.93607 factor:1 | -1 (0.37576) | -1 | -1 |
| G: -5052.27415 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11316.24044 HOMO: -5.49670 LUMO: 0.27211 factor:1 | -1 (0.39941) | -1 | -1 |
| G: -5052.27415 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11316.24634 HOMO: -5.68990 LUMO: 0.24218 factor:1 | -1 (0.39350) | -1 | -1 |
| G: -5052.27415 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11316.74978 HOMO: -5.68174 LUMO: 0.69933 factor:1 | 1 (-0.10993) | -1 | -1 |
| G: -5052.27415 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11316.84254 HOMO: -5.28173 LUMO: 1.00954 factor:1 | 1 (-0.20270) | -1 | -1 |
| G: -5052.27415 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11316.61467 HOMO: -5.94025 LUMO: 0.73471 factor:1 | -1 (0.02517) | -1 | -1 |
| G: -5052.27415 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11317.24067 HOMO: -5.65725 LUMO: 1.28710 factor:1 | 1 (-0.60083) | -1 | -1 |
| G: -5052.27415 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11316.94244 HOMO: -5.41507 LUMO: 0.87076 factor:1 | 1 (-0.30259) | -1 | -1 |
| G: -5052.27415 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11316.27116 HOMO: -5.96474 LUMO: 0.29660 factor:1 | -1 (0.36869) | -1 | -1 |
| G: -5052.27415 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11317.15009 HOMO: -7.00421 LUMO: 0.08708 factor:1 | 1 (-0.51024) | -1 | -1 |
| G: -5052.27415 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11317.00883 HOMO: -5.40418 LUMO: 0.90070 factor:1 | 1 (-0.36899) | -1 | -1 |
| G: -5052.27415 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11317.17452 HOMO: -7.00421 LUMO: -0.30477 factor:1 | 1 (-0.53468) | -1 | -1 |
| G: -5052.27415 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11316.66768 HOMO: -5.85861 LUMO: 0.74015 factor:1 | 1 (-0.02784) | -1 | -1 |
| G: -5052.27415 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11316.31494 HOMO: -5.71439 LUMO: 0.26395 factor:1 | -1 (0.32490) | -1 | -1 |
| G: -5052.27415 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11315.89711 HOMO: -7.13755 LUMO: -0.78369 factor:1 | -1 (0.74273) | 1 | -1 |
| G: -5052.27415 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11315.95975 HOMO: -7.31442 LUMO: -0.98233 factor:1 | -1 (0.68009) | 1 | -1 |
| G: -5052.27415 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11315.91741 HOMO: -7.25728 LUMO: -1.00410 factor:1 | -1 (0.72244) | 1 | -1 |
| G: -5052.27415 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11316.51364 HOMO: -7.48585 LUMO: -0.83811 factor:1 | -1 (0.12621) | 1 | -1 |
| G: -5052.27415 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11316.47957 HOMO: -7.24911 LUMO: -0.77280 factor:1 | -1 (0.16028) | 1 | -1 |
| G: -5052.27415 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11315.45386 HOMO: -7.55116 LUMO: -1.19730 factor:1 | -1 (1.18598) | 1 | -1 |
| G: -5052.27415 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11316.66406 HOMO: -5.76881 LUMO: 0.28028 factor:1 | 1 (-0.02422) | -1 | -1 |
| G: -5052.27415 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11316.40373 HOMO: -5.77153 LUMO: -0.26939 factor:1 | -1 (0.23611) | -1 | -1 |
| G: -5052.27415 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11316.64153 HOMO: -5.82868 LUMO: 0.36735 factor:1 | 1 (-0.00169) | -1 | -1 |
| G: -5052.27415 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11316.42387 HOMO: -5.83140 LUMO: -0.17960 factor:1 | -1 (0.21598) | -1 | -1 |
| G: -5052.27415 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11316.64322 HOMO: -6.28855 LUMO: 0.01088 factor:1 | 1 (-0.00337) | -1 | -1 |
| G: -5052.27415 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11316.51108 HOMO: -6.31576 LUMO: 0.25307 factor:1 | -1 (0.12876) | -1 | -1 |
| G: -5052.27415 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11316.14819 HOMO: -7.06408 LUMO: -2.76196 factor:1 | -1 (0.49166) | -1 | -1 |
| G: -5052.27415 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11316.73049 HOMO: -5.95657 LUMO: 0.37552 factor:1 | 1 (-0.09064) | -1 | -1 |
| G: -5052.27415 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11316.65751 HOMO: -6.61781 LUMO: 0.02721 factor:1 | 1 (-0.01766) | -1 | -1 |
| G: -5052.27415 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11316.77993 HOMO: -6.26678 LUMO: -0.66668 factor:1 | 1 (-0.14008) | -1 | -1 |
| G: -5052.27415 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11316.47870 HOMO: -6.00011 LUMO: -0.13334 factor:1 | -1 (0.16115) | -1 | -1 |
| G: -5052.27415 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11317.04374 HOMO: -5.60555 LUMO: 0.67484 factor:1 | 1 (-0.40390) | -1 | -1 |
| G: -5052.27415 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11317.30527 HOMO: -5.79875 LUMO: 0.99049 factor:1 | 1 (-0.66543) | -1 | -1 |
| G: -5052.27415 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11317.38930 HOMO: -5.97834 LUMO: 0.48436 factor:1 | 1 (-0.74946) | -1 | -1 |
| G: -5052.27415 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11317.30435 HOMO: -5.82868 LUMO: 0.91974 factor:1 | 1 (-0.66450) | -1 | -1 |
| G: -5052.27415 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11317.18573 HOMO: -5.86677 LUMO: 0.99594 factor:1 | 1 (-0.54589) | -1 | -1 |
| G: -5052.27415 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11317.19248 HOMO: -5.70079 LUMO: 0.48980 factor:1 | 1 (-0.55264) | -1 | -1 |
| G: -5052.27415 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11316.26484 HOMO: -7.39605 LUMO: -1.02315 factor:1 | -1 (0.37500) | 1 | -1 |
| G: -5052.27415 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11316.19818 HOMO: -7.22734 LUMO: -1.12927 factor:1 | -1 (0.44167) | 1 | -1 |
| G: -5052.27415 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11316.92238 HOMO: -7.58926 LUMO: -0.65035 factor:1 | 1 (-0.28254) | 1 | 1 |
| G: -5052.27415 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11316.85520 HOMO: -7.43959 LUMO: -0.75648 factor:1 | 1 (-0.21535) | 1 | 1 |
| G: -5052.27415 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11315.74353 HOMO: -7.55388 LUMO: -1.15104 factor:1 | -1 (0.89632) | 1 | -1 |
| G: -5187.86552 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11454.13101 HOMO: -6.74570 LUMO: -2.85447 factor:1 | 1 (-1.89979) | -1 | -1 |
| G: -5187.86552 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11454.48943 HOMO: -7.35524 LUMO: -1.25444 factor:1 | 1 (-2.25822) | 1 | 1 |
| G: -5187.86552 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11453.97329 HOMO: -6.81645 LUMO: -1.20819 factor:1 | 1 (-1.74207) | -1 | -1 |
| G: -5187.86552 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11454.46405 HOMO: -6.99605 LUMO: -1.62996 factor:1 | 1 (-2.23283) | -1 | -1 |
| G: -5187.86552 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11455.20512 HOMO: -6.88992 LUMO: -0.47620 factor:1 | 1 (-2.97391) | -1 | -1 |
| G: -5187.86552 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11454.41994 HOMO: -7.22190 LUMO: -0.01905 factor:1 | 1 (-2.18872) | 1 | 1 |
| G: -5187.86552 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11453.56871 HOMO: -6.77836 LUMO: -0.82995 factor:1 | 1 (-1.33749) | -1 | -1 |
| G: -5187.86552 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11453.48057 HOMO: -6.48447 LUMO: -0.95512 factor:1 | 1 (-1.24936) | -1 | -1 |
| G: -5187.86552 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11455.33122 HOMO: -7.81239 LUMO: 1.22179 factor:1 | 1 (-3.10000) | 1 | 1 |
| G: -5187.86552 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11455.02667 HOMO: -7.36612 LUMO: 0.19320 factor:1 | 1 (-2.79545) | 1 | 1 |
| G: -5187.86552 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11454.84136 HOMO: -7.24095 LUMO: 0.33470 factor:1 | 1 (-2.61014) | 1 | 1 |
| G: -5187.86552 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11454.71349 HOMO: -7.15932 LUMO: -2.24222 factor:1 | 1 (-2.48228) | -1 | -1 |
| G: -5187.86552 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11454.07242 HOMO: -6.88992 LUMO: -2.69937 factor:1 | 1 (-1.84120) | -1 | -1 |
| G: -5187.86552 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11454.38579 HOMO: -6.97428 LUMO: -0.98233 factor:1 | 1 (-2.15457) | -1 | -1 |
| G: -5187.86552 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11455.00509 HOMO: -7.17564 LUMO: -0.93879 factor:1 | 1 (-2.77387) | 1 | 1 |
| G: -5187.86552 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11454.33251 HOMO: -6.81645 LUMO: -1.14288 factor:1 | 1 (-2.10129) | -1 | -1 |
| G: -5187.86552 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11455.09478 HOMO: -6.83006 LUMO: -0.63403 factor:1 | 1 (-2.86356) | -1 | -1 |
| G: -5187.86552 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11453.37135 HOMO: -7.17292 LUMO: -1.07213 factor:1 | 1 (-1.14013) | 1 | 1 |
| G: -5187.86552 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11454.40301 HOMO: -7.53755 LUMO: 0.15510 factor:1 | 1 (-2.17180) | 1 | 1 |
| G: -5187.86552 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11453.54419 HOMO: -6.50080 LUMO: -0.51702 factor:1 | 1 (-1.31298) | -1 | -1 |
| G: -5187.86552 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11453.40027 HOMO: -6.72665 LUMO: -0.80001 factor:1 | 1 (-1.16906) | -1 | -1 |
| G: -5187.86552 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11451.84998 HOMO: -6.72665 LUMO: 1.68711 factor:1 | -1 (0.38123) | -1 | -1 |
| G: -5187.86552 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11454.82016 HOMO: -7.11850 LUMO: -0.75103 factor:1 | 1 (-2.58895) | 1 | 1 |
| G: -5187.86552 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11453.85092 HOMO: -6.87087 LUMO: -0.85988 factor:1 | 1 (-1.61970) | -1 | -1 |
| G: -5187.86552 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11454.89660 HOMO: -7.08857 LUMO: -0.89798 factor:1 | 1 (-2.66538) | 1 | 1 |
| G: -5187.86552 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11453.02024 HOMO: -6.71305 LUMO: -0.85444 factor:1 | 1 (-0.78902) | -1 | -1 |
| G: -5187.86552 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11453.13325 HOMO: -6.59332 LUMO: -0.60137 factor:1 | 1 (-0.90203) | -1 | -1 |
| G: -5187.86552 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11453.59198 HOMO: -7.28993 LUMO: 0.03265 factor:1 | 1 (-1.36076) | 1 | 1 |
| G: -5187.86552 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11454.84269 HOMO: -7.32258 LUMO: 0.13878 factor:1 | 1 (-2.61148) | 1 | 1 |
| G: -5187.86552 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11454.86462 HOMO: -7.28993 LUMO: 0.11429 factor:1 | 1 (-2.63341) | 1 | 1 |
| G: -5187.86552 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11453.98975 HOMO: -6.86271 LUMO: -1.03947 factor:1 | 1 (-1.75854) | -1 | -1 |
| G: -5187.86552 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11453.56114 HOMO: -6.55794 LUMO: -0.84900 factor:1 | 1 (-1.32993) | -1 | -1 |
| G: -5187.86552 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11454.38682 HOMO: -7.03686 LUMO: 0.11429 factor:1 | 1 (-2.15560) | -1 | -1 |
| G: -5187.86552 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11454.51564 HOMO: -7.06952 LUMO: -0.96056 factor:1 | 1 (-2.28442) | 1 | 1 |
| G: -5187.86552 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11453.91897 HOMO: -6.90897 LUMO: -0.99866 factor:1 | 1 (-1.68776) | -1 | -1 |
| G: -5187.86552 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11454.89616 HOMO: -7.00693 LUMO: -0.83539 factor:1 | 1 (-2.66495) | -1 | -1 |
| G: -5187.86552 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11453.83489 HOMO: -6.74298 LUMO: -0.85172 factor:1 | 1 (-1.60368) | -1 | -1 |
| G: -5187.86552 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11454.12189 HOMO: -6.83822 LUMO: -1.07213 factor:1 | 1 (-1.89067) | -1 | -1 |
| G: -5187.86552 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11454.29610 HOMO: -7.21918 LUMO: -1.55377 factor:1 | 1 (-2.06488) | 1 | 1 |
| G: -5187.86552 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11454.34377 HOMO: -6.84094 LUMO: -1.09934 factor:1 | 1 (-2.11256) | -1 | -1 |
| G: -5187.86552 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11454.81896 HOMO: -7.09129 LUMO: -0.85988 factor:1 | 1 (-2.58775) | 1 | 1 |
| G: -5187.86552 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11454.34655 HOMO: -6.57971 LUMO: -2.27215 factor:1 | 1 (-2.11533) | -1 | -1 |
| G: -5187.86552 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11454.97290 HOMO: -6.81373 LUMO: -1.86942 factor:1 | 1 (-2.74168) | -1 | -1 |
| G: -5187.86552 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11453.98303 HOMO: -6.59060 LUMO: -2.30480 factor:1 | 1 (-1.75181) | -1 | -1 |
| G: -5187.86552 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11454.51651 HOMO: -6.72938 LUMO: -1.23540 factor:1 | 1 (-2.28529) | -1 | -1 |
| G: -5187.86552 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11454.48965 HOMO: -6.94707 LUMO: -2.62318 factor:1 | 1 (-2.25844) | -1 | -1 |
| G: -5187.86552 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11453.46552 HOMO: -7.28177 LUMO: -0.09796 factor:1 | 1 (-1.23431) | 1 | 1 |
| G: -5187.86552 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11452.95605 HOMO: -6.80013 LUMO: -0.79729 factor:1 | 1 (-0.72483) | -1 | -1 |
| G: -5187.86552 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11453.56626 HOMO: -7.26544 LUMO: 0.12789 factor:1 | 1 (-1.33505) | 1 | 1 |
| G: -5187.86552 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11453.05986 HOMO: -6.51713 LUMO: -0.49253 factor:1 | 1 (-0.82864) | -1 | -1 |
| G: -5187.86552 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11453.22979 HOMO: -6.68856 LUMO: -0.77280 factor:1 | 1 (-0.99858) | -1 | -1 |
| G: -5187.86552 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11453.56555 HOMO: -6.41100 LUMO: -0.70750 factor:1 | 1 (-1.33434) | -1 | -1 |
| G: -5187.86552 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11454.38698 HOMO: -7.56204 LUMO: 0.22041 factor:1 | 1 (-2.15577) | 1 | 1 |
| G: -5187.86552 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11451.45253 HOMO: -6.68312 LUMO: 1.30343 factor:1 | -1 (0.77868) | -1 | -1 |
| G: -5187.86552 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11454.69300 HOMO: -7.24367 LUMO: 0.17415 factor:1 | 1 (-2.46179) | 1 | 1 |
| G: -5187.86552 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11455.00738 HOMO: -7.52395 LUMO: 1.16737 factor:1 | 1 (-2.77616) | 1 | 1 |
| G: -5187.86552 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11454.47066 HOMO: -6.89264 LUMO: 0.23130 factor:1 | 1 (-2.23944) | -1 | -1 |
| G: -5187.86552 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11454.79004 HOMO: -7.21102 LUMO: 0.19048 factor:1 | 1 (-2.55882) | 1 | 1 |
| G: -5187.86552 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11454.62927 HOMO: -7.08312 LUMO: 0.25034 factor:1 | 1 (-2.39806) | 1 | 1 |
| G: -5187.86552 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11453.87359 HOMO: -6.49536 LUMO: -0.65852 factor:1 | 1 (-1.64237) | -1 | -1 |
| G: -5187.86552 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11453.87288 HOMO: -6.85455 LUMO: 0.13606 factor:1 | 1 (-1.64166) | -1 | -1 |
| G: -5187.86552 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11454.83094 HOMO: -7.10217 LUMO: 0.35919 factor:1 | 1 (-2.59972) | 1 | 1 |
| G: -5187.86552 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11455.29418 HOMO: -7.77429 LUMO: 1.19186 factor:1 | 1 (-3.06297) | 1 | 1 |
| G: -5187.86552 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11454.26584 HOMO: -6.57427 LUMO: -0.50069 factor:1 | 1 (-2.03462) | -1 | -1 |
| G: -5187.86552 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11454.91271 HOMO: -7.36340 LUMO: 0.10068 factor:1 | 1 (-2.68149) | 1 | 1 |
| G: -5187.86552 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11455.02501 HOMO: -7.28177 LUMO: 0.15238 factor:1 | 1 (-2.79379) | 1 | 1 |
| G: -5187.86552 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11454.16037 HOMO: -6.86543 LUMO: -0.84355 factor:1 | 1 (-1.92915) | -1 | -1 |
| G: -5187.86552 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11452.06833 HOMO: -6.55794 LUMO: 1.39594 factor:1 | -1 (0.16289) | -1 | -1 |
| G: -5187.86552 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11452.26863 HOMO: -6.26134 LUMO: 1.53744 factor:1 | 1 (-0.03742) | -1 | -1 |
| G: -5187.86552 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11451.90373 HOMO: -5.97562 LUMO: 1.42316 factor:1 | -1 (0.32749) | -1 | -1 |
| G: -5187.86552 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11452.82625 HOMO: -6.65046 LUMO: 1.44492 factor:1 | 1 (-0.59503) | -1 | -1 |
| G: -5187.86552 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11453.90436 HOMO: -6.92258 LUMO: 0.17415 factor:1 | 1 (-1.67315) | -1 | -1 |
| G: -5187.86552 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11453.66509 HOMO: -7.40966 LUMO: 0.19592 factor:1 | 1 (-1.43388) | 1 | 1 |
| G: -5187.86552 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11453.90877 HOMO: -7.17564 LUMO: 0.16871 factor:1 | 1 (-1.67755) | 1 | 1 |
| G: -5187.86552 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11454.18200 HOMO: -7.46953 LUMO: 0.22313 factor:1 | 1 (-1.95078) | 1 | 1 |
| G: -5187.86552 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11452.22803 HOMO: -6.13345 LUMO: 1.85854 factor:1 | -1 (0.00318) | -1 | -1 |
| G: -5187.86552 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11453.85764 HOMO: -6.99333 LUMO: -1.65717 factor:1 | 1 (-1.62642) | -1 | -1 |
| G: -5187.86552 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11453.89457 HOMO: -6.93074 LUMO: -1.79323 factor:1 | 1 (-1.66335) | -1 | -1 |
| G: -5187.86552 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11453.56689 HOMO: -6.87904 LUMO: -1.79323 factor:1 | 1 (-1.33567) | -1 | -1 |
| G: -5187.86552 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11452.13391 HOMO: -6.84094 LUMO: 0.66940 factor:1 | -1 (0.09731) | -1 | -1 |
| G: -5187.86552 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11454.03109 HOMO: -7.13210 LUMO: -1.17553 factor:1 | 1 (-1.79987) | 1 | 1 |
| G: -5187.86552 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11454.20924 HOMO: -6.52801 LUMO: -2.23678 factor:1 | 1 (-1.97802) | -1 | -1 |
| G: -5187.86552 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11454.87532 HOMO: -6.81917 LUMO: -1.86398 factor:1 | 1 (-2.64410) | -1 | -1 |
| G: -5187.86552 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11454.22238 HOMO: -7.30626 LUMO: -1.66806 factor:1 | 1 (-1.99117) | 1 | 1 |
| G: -5187.86552 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11454.21514 HOMO: -6.98516 LUMO: -1.40683 factor:1 | 1 (-1.98393) | -1 | -1 |
| G: -5187.86552 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11454.77537 HOMO: -6.95523 LUMO: -0.97145 factor:1 | 1 (-2.54416) | -1 | -1 |
| G: -5187.86552 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11453.93163 HOMO: -6.83278 LUMO: -2.68848 factor:1 | 1 (-1.70041) | -1 | -1 |
| G: -5187.86552 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11454.08031 HOMO: -7.25456 LUMO: -2.97420 factor:1 | 1 (-1.84910) | -1 | -1 |
| G: -5187.86552 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11453.61462 HOMO: -6.80557 LUMO: -2.65039 factor:1 | 1 (-1.38340) | -1 | -1 |
| G: -5187.86552 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11452.06354 HOMO: -7.10489 LUMO: 0.77008 factor:1 | -1 (0.16768) | 1 | -1 |
| G: -5187.86552 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11454.46840 HOMO: -7.28993 LUMO: -1.06124 factor:1 | 1 (-2.23718) | 1 | 1 |
| G: -5187.86552 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11453.66841 HOMO: -7.11578 LUMO: -1.10206 factor:1 | 1 (-1.43720) | 1 | 1 |
| G: -5187.86552 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11454.01854 HOMO: -6.91713 LUMO: -1.36329 factor:1 | 1 (-1.78733) | -1 | -1 |
| G: -5187.86552 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11452.24605 HOMO: -7.07224 LUMO: 0.51974 factor:1 | 1 (-0.01483) | 1 | 1 |
| G: -5187.86552 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11454.66484 HOMO: -7.22734 LUMO: -0.93335 factor:1 | 1 (-2.43362) | 1 | 1 |
| G: -5187.86552 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11454.86495 HOMO: -7.19469 LUMO: -0.96600 factor:1 | 1 (-2.63374) | 1 | 1 |
| G: -5187.86552 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11454.81034 HOMO: -6.93890 LUMO: -0.66940 factor:1 | 1 (-2.57912) | -1 | -1 |
| G: -5187.86552 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11454.23547 HOMO: -7.09673 LUMO: -1.05852 factor:1 | 1 (-2.00425) | 1 | 1 |
| G: -5187.86552 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11454.59564 HOMO: -7.19197 LUMO: -2.26943 factor:1 | 1 (-2.36442) | -1 | -1 |
| G: -5187.86552 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11453.70882 HOMO: -6.90081 LUMO: -2.64767 factor:1 | 1 (-1.47761) | -1 | -1 |
| G: -5187.86552 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11453.73677 HOMO: -6.93890 LUMO: -2.65039 factor:1 | 1 (-1.50555) | -1 | -1 |
| G: -5187.86552 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11453.74368 HOMO: -6.80013 LUMO: -2.54154 factor:1 | 1 (-1.51246) | -1 | -1 |
| G: -5187.86552 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11453.17409 HOMO: -6.68040 LUMO: -0.89798 factor:1 | 1 (-0.94287) | -1 | -1 |
| G: -5187.86552 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11453.14993 HOMO: -7.01782 LUMO: -1.09662 factor:1 | 1 (-0.91871) | -1 | -1 |
| G: -5187.86552 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11453.34051 HOMO: -6.58516 LUMO: -0.83539 factor:1 | 1 (-1.10930) | -1 | -1 |
| G: -5187.86552 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11454.17354 HOMO: -7.46953 LUMO: 0.06259 factor:1 | 1 (-1.94232) | 1 | 1 |
| G: -5187.86552 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11453.38098 HOMO: -6.96884 LUMO: -0.99866 factor:1 | 1 (-1.14976) | -1 | -1 |
| G: -5187.86552 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11454.18135 HOMO: -7.29809 LUMO: -0.19320 factor:1 | 1 (-1.95013) | 1 | 1 |
| G: -5187.86552 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11453.87897 HOMO: -6.86271 LUMO: 0.04082 factor:1 | 1 (-1.64776) | -1 | -1 |
| G: -5187.86552 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11453.54852 HOMO: -6.36746 LUMO: -1.02587 factor:1 | 1 (-1.31730) | -1 | -1 |
| G: -5187.86552 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11453.07118 HOMO: -7.15659 LUMO: -1.25989 factor:1 | 1 (-0.83996) | 1 | 1 |
| G: -5187.86552 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11453.11205 HOMO: -6.69128 LUMO: -0.59865 factor:1 | 1 (-0.88083) | -1 | -1 |
| G: -5187.86552 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11453.16288 HOMO: -7.09129 LUMO: -1.08573 factor:1 | 1 (-0.93166) | 1 | 1 |
| G: -5187.86552 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11452.91825 HOMO: -6.64502 LUMO: -0.66396 factor:1 | 1 (-0.68703) | -1 | -1 |
| G: -5187.86552 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11453.17344 HOMO: -6.93346 LUMO: -0.87349 factor:1 | 1 (-0.94222) | -1 | -1 |
| G: -5187.86552 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11453.73709 HOMO: -6.77019 LUMO: -0.87349 factor:1 | 1 (-1.50588) | -1 | -1 |
| G: -5187.86552 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11453.81062 HOMO: -6.59060 LUMO: -0.82995 factor:1 | 1 (-1.57940) | -1 | -1 |
| G: -5187.86552 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11453.82251 HOMO: -7.17564 LUMO: -1.08846 factor:1 | 1 (-1.59129) | 1 | 1 |
| G: -5187.86552 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11453.13991 HOMO: -7.27088 LUMO: -1.18642 factor:1 | 1 (-0.90870) | 1 | 1 |
| G: -5187.86552 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11453.12680 HOMO: -7.06680 LUMO: -1.13199 factor:1 | 1 (-0.89558) | 1 | 1 |
| G: -5187.86552 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11453.37110 HOMO: -7.21918 LUMO: -1.03947 factor:1 | 1 (-1.13988) | 1 | 1 |
| G: -5187.86552 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11453.85206 HOMO: -7.26000 LUMO: -0.11973 factor:1 | 1 (-1.62085) | 1 | 1 |
| G: -5187.86552 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11453.97266 HOMO: -6.77564 LUMO: 0.23402 factor:1 | 1 (-1.74145) | -1 | -1 |
| G: -5187.86552 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11453.46022 HOMO: -7.07224 LUMO: -0.75648 factor:1 | 1 (-1.22900) | 1 | 1 |
| G: -5187.86552 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11453.58934 HOMO: -7.45048 LUMO: 0.18232 factor:1 | 1 (-1.35812) | 1 | 1 |
| G: -5187.86552 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11453.60444 HOMO: -7.48313 LUMO: 0.15238 factor:1 | 1 (-1.37322) | 1 | 1 |
| G: -5187.86552 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11453.11586 HOMO: -6.60692 LUMO: -0.50885 factor:1 | 1 (-0.88464) | -1 | -1 |
| G: -5187.86552 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11453.26615 HOMO: -6.62869 LUMO: -0.60954 factor:1 | 1 (-1.03493) | -1 | -1 |
| G: -5187.86552 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11454.42002 HOMO: -7.40422 LUMO: -1.28982 factor:1 | 1 (-2.18880) | 1 | 1 |
| G: -5187.86552 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11453.59154 HOMO: -6.75114 LUMO: -1.23268 factor:1 | 1 (-1.36032) | -1 | -1 |
| G: -5187.86552 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11453.87116 HOMO: -6.84638 LUMO: -0.73199 factor:1 | 1 (-1.63995) | -1 | -1 |
| G: -5187.86552 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11453.66841 HOMO: -6.79196 LUMO: -1.43676 factor:1 | 1 (-1.43720) | -1 | -1 |
| G: -5187.86552 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11453.59919 HOMO: -7.00965 LUMO: -1.37690 factor:1 | 1 (-1.36797) | -1 | -1 |
| G: -5187.86552 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11453.70188 HOMO: -6.97972 LUMO: -1.58098 factor:1 | 1 (-1.47067) | -1 | -1 |
| G: -5187.86552 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11453.83073 HOMO: -6.91169 LUMO: -1.48574 factor:1 | 1 (-1.59951) | -1 | -1 |
| G: -5187.86552 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11454.15797 HOMO: -6.90081 LUMO: -1.30343 factor:1 | 1 (-1.92676) | -1 | -1 |
| G: -5187.86552 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11453.79266 HOMO: -6.78652 LUMO: -1.51840 factor:1 | 1 (-1.56144) | -1 | -1 |
| G: -5187.86552 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11452.58510 HOMO: -6.84638 LUMO: -1.15104 factor:1 | 1 (-0.35388) | -1 | -1 |
| G: -5187.86552 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11452.93809 HOMO: -6.61237 LUMO: -0.89798 factor:1 | 1 (-0.70687) | -1 | -1 |
| G: -5187.86552 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11452.89716 HOMO: -7.16204 LUMO: -1.30070 factor:1 | 1 (-0.66594) | 1 | 1 |
| G: -5187.86552 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11453.51361 HOMO: -7.32803 LUMO: 0.14694 factor:1 | 1 (-1.28239) | 1 | 1 |
| G: -5187.86552 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11453.01509 HOMO: -6.99877 LUMO: -0.87621 factor:1 | 1 (-0.78388) | -1 | -1 |
| G: -5187.86552 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11452.67291 HOMO: -6.99877 LUMO: -0.97145 factor:1 | 1 (-0.44170) | -1 | -1 |
| G: -5187.86552 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11452.96688 HOMO: -7.08040 LUMO: -1.09662 factor:1 | 1 (-0.73566) | 1 | 1 |
| G: -5187.86552 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11453.05518 HOMO: -6.90897 LUMO: -1.14016 factor:1 | 1 (-0.82396) | -1 | -1 |
| G: -5187.86552 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11452.83798 HOMO: -6.68312 LUMO: -0.74831 factor:1 | 1 (-0.60676) | -1 | -1 |
| G: -5187.86552 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11453.11980 HOMO: -6.99061 LUMO: -0.86804 factor:1 | 1 (-0.88859) | -1 | -1 |
| G: -5187.86552 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11453.14721 HOMO: -7.10761 LUMO: -1.18642 factor:1 | 1 (-0.91599) | 1 | 1 |
| G: -5187.86552 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11453.27850 HOMO: -6.79196 LUMO: -0.71294 factor:1 | 1 (-1.04728) | -1 | -1 |
| G: -5187.86552 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11452.93749 HOMO: -6.86271 LUMO: -0.81362 factor:1 | 1 (-0.70627) | -1 | -1 |
| G: -5187.86552 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11453.44280 HOMO: -7.01510 LUMO: -0.99322 factor:1 | 1 (-1.21159) | -1 | -1 |
| G: -5187.86552 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11453.55078 HOMO: -6.88720 LUMO: -0.87893 factor:1 | 1 (-1.31956) | -1 | -1 |
| G: -5187.86552 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11454.46162 HOMO: -6.88448 LUMO: 0.22041 factor:1 | 1 (-2.23041) | -1 | -1 |
| G: -5187.86552 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11454.87535 HOMO: -7.55932 LUMO: 1.12111 factor:1 | 1 (-2.64413) | 1 | 1 |
| G: -5187.86552 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11453.97024 HOMO: -6.46815 LUMO: -0.86260 factor:1 | 1 (-1.73903) | -1 | -1 |
| G: -5187.86552 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11454.57817 HOMO: -7.13755 LUMO: 0.23130 factor:1 | 1 (-2.34695) | 1 | 1 |
| G: -5187.86552 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11451.63480 HOMO: -6.78924 LUMO: 1.51023 factor:1 | -1 (0.59642) | -1 | -1 |
| G: -5187.86552 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11451.80723 HOMO: -6.48992 LUMO: 1.74969 factor:1 | -1 (0.42398) | -1 | -1 |
| G: -5187.86552 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11452.42088 HOMO: -6.78380 LUMO: 1.81500 factor:1 | 1 (-0.18966) | -1 | -1 |
| G: -5187.86552 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11452.33881 HOMO: -6.49536 LUMO: 1.70615 factor:1 | 1 (-0.10759) | -1 | -1 |
| G: -5187.86552 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11452.50338 HOMO: -6.38651 LUMO: 1.44492 factor:1 | 1 (-0.27217) | -1 | -1 |
| G: -5187.86552 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11453.39118 HOMO: -6.83822 LUMO: 1.38234 factor:1 | 1 (-1.15997) | -1 | -1 |
| G: -5187.86552 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11451.94599 HOMO: -6.01644 LUMO: 1.20274 factor:1 | -1 (0.28523) | -1 | -1 |
| G: -5187.86552 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11452.23522 HOMO: -6.18243 LUMO: 1.77962 factor:1 | 1 (-0.00400) | -1 | -1 |
| G: -5187.86552 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11453.02791 HOMO: -6.81917 LUMO: -1.01771 factor:1 | 1 (-0.79669) | -1 | -1 |
| G: -5187.86552 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11453.69745 HOMO: -6.61237 LUMO: -0.91702 factor:1 | 1 (-1.46623) | -1 | -1 |
| G: -5187.86552 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11453.77884 HOMO: -6.84094 LUMO: -0.84900 factor:1 | 1 (-1.54762) | -1 | -1 |
| G: -5187.86552 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11453.67761 HOMO: -6.81917 LUMO: -1.01771 factor:1 | 1 (-1.44639) | -1 | -1 |
| G: -5187.86552 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11455.18746 HOMO: -7.86953 LUMO: 1.16737 factor:1 | 1 (-2.95624) | 1 | 1 |
| G: -5187.86552 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11454.82900 HOMO: -7.40694 LUMO: 0.11429 factor:1 | 1 (-2.59779) | 1 | 1 |
| G: -5187.86552 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11454.01805 HOMO: -6.70489 LUMO: -0.65035 factor:1 | 1 (-1.78684) | -1 | -1 |
| G: -5187.86552 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11454.83937 HOMO: -7.23279 LUMO: 0.33470 factor:1 | 1 (-2.60816) | 1 | 1 |
| G: -5187.86552 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11454.45969 HOMO: -7.17020 LUMO: 0.41361 factor:1 | 1 (-2.22848) | 1 | 1 |
| G: -5187.86552 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11453.94257 HOMO: -6.90353 LUMO: -0.90070 factor:1 | 1 (-1.71135) | -1 | -1 |
| G: -5187.86552 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11454.79869 HOMO: -7.39061 LUMO: 0.17687 factor:1 | 1 (-2.56748) | 1 | 1 |
| G: -5187.86552 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11454.66443 HOMO: -7.16748 LUMO: 0.42178 factor:1 | 1 (-2.43321) | 1 | 1 |
| G: -5187.86552 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11453.03071 HOMO: -7.36884 LUMO: -1.11295 factor:1 | 1 (-0.79950) | 1 | 1 |
| G: -5187.86552 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11453.78175 HOMO: -7.33347 LUMO: 0.33198 factor:1 | 1 (-1.55053) | 1 | 1 |
| G: -5187.86552 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11453.22489 HOMO: -7.31986 LUMO: -0.83539 factor:1 | 1 (-0.99368) | 1 | 1 |
| G: -5187.86552 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11453.83957 HOMO: -7.31170 LUMO: 0.08708 factor:1 | 1 (-1.60836) | 1 | 1 |
| G: -5187.86552 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11453.89857 HOMO: -7.36884 LUMO: 0.38096 factor:1 | 1 (-1.66735) | 1 | 1 |
| G: -5187.86552 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11451.42557 HOMO: -6.99333 LUMO: 1.74153 factor:1 | -1 (0.80565) | -1 | -1 |
| G: -5187.86552 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11452.18874 HOMO: -6.94435 LUMO: 1.74969 factor:1 | -1 (0.04248) | -1 | -1 |
| G: -5187.86552 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11452.34186 HOMO: -7.02598 LUMO: 1.43404 factor:1 | 1 (-0.11064) | -1 | -1 |
| G: -5187.86552 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11451.88936 HOMO: -6.41100 LUMO: 1.62996 factor:1 | -1 (0.34186) | -1 | -1 |
| G: -5187.86552 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11452.24411 HOMO: -6.57699 LUMO: 1.81228 factor:1 | 1 (-0.01290) | -1 | -1 |
| G: -5187.86552 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11452.05246 HOMO: -6.86543 LUMO: 1.49935 factor:1 | -1 (0.17875) | -1 | -1 |
| G: -5187.86552 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11453.17983 HOMO: -6.91169 LUMO: -1.22451 factor:1 | 1 (-0.94862) | -1 | -1 |
| G: -5187.86552 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11453.35548 HOMO: -7.09945 LUMO: -1.23812 factor:1 | 1 (-1.12427) | 1 | 1 |
| G: -5187.86552 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11454.22355 HOMO: -7.48857 LUMO: 0.10340 factor:1 | 1 (-1.99234) | 1 | 1 |
| G: -5187.86552 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11454.22554 HOMO: -7.21918 LUMO: -0.06803 factor:1 | 1 (-1.99432) | 1 | 1 |
| G: -5187.86552 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11453.15023 HOMO: -6.34025 LUMO: -0.68845 factor:1 | 1 (-0.91901) | -1 | -1 |
| G: -5187.86552 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11453.32041 HOMO: -6.82734 LUMO: -0.77825 factor:1 | 1 (-1.08919) | -1 | -1 |
| G: -5187.86552 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11453.38416 HOMO: -6.92258 LUMO: -1.03675 factor:1 | 1 (-1.15295) | -1 | -1 |
| G: -5187.86552 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11453.07050 HOMO: -6.42461 LUMO: -0.95240 factor:1 | 1 (-0.83928) | -1 | -1 |
| G: -5187.86552 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11453.40941 HOMO: -6.96067 LUMO: -1.05036 factor:1 | 1 (-1.17820) | -1 | -1 |
| G: -5187.86552 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11454.52280 HOMO: -7.23551 LUMO: 0.12245 factor:1 | 1 (-2.29158) | 1 | 1 |
| G: -5187.86552 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11454.43708 HOMO: -6.85183 LUMO: 0.16055 factor:1 | 1 (-2.20586) | -1 | -1 |
| G: -5187.86552 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11453.87495 HOMO: -6.46815 LUMO: -0.89253 factor:1 | 1 (-1.64373) | -1 | -1 |
| G: -5187.86552 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11454.66974 HOMO: -7.23823 LUMO: -0.06259 factor:1 | 1 (-2.43852) | 1 | 1 |
| G: -5187.86552 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11453.97321 HOMO: -6.76475 LUMO: -0.99049 factor:1 | 1 (-1.74199) | -1 | -1 |
| G: -5187.86552 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11454.08687 HOMO: -7.14843 LUMO: -0.88165 factor:1 | 1 (-1.85565) | 1 | 1 |
| G: -5187.86552 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11454.27710 HOMO: -7.15659 LUMO: 0.20681 factor:1 | 1 (-2.04589) | 1 | 1 |
| G: -5187.86552 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11454.01400 HOMO: -7.11306 LUMO: 0.14150 factor:1 | 1 (-1.78278) | 1 | 1 |
| G: -5187.86552 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11453.56966 HOMO: -6.67223 LUMO: -0.86260 factor:1 | 1 (-1.33845) | -1 | -1 |
| G: -5187.86552 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11454.12450 HOMO: -6.92530 LUMO: 0.30749 factor:1 | 1 (-1.89329) | -1 | -1 |
| G: -5187.86552 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11453.53312 HOMO: -6.50624 LUMO: -0.70477 factor:1 | 1 (-1.30190) | -1 | -1 |
| G: -5187.86552 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11454.56693 HOMO: -7.35524 LUMO: 0.75103 factor:1 | 1 (-2.33572) | 1 | 1 |
| G: -5187.86552 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11453.50963 HOMO: -7.07768 LUMO: -0.26939 factor:1 | 1 (-1.27842) | 1 | 1 |
| G: -5187.86552 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11454.76253 HOMO: -7.15932 LUMO: 0.42450 factor:1 | 1 (-2.53131) | 1 | 1 |
| G: -5187.86552 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11454.76215 HOMO: -7.46136 LUMO: 0.04626 factor:1 | 1 (-2.53093) | 1 | 1 |
| G: -5187.86552 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11453.98191 HOMO: -7.05047 LUMO: -1.06669 factor:1 | 1 (-1.75070) | -1 | -1 |
| G: -5187.86552 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11454.14660 HOMO: -6.66951 LUMO: -0.99322 factor:1 | 1 (-1.91538) | -1 | -1 |
| G: -5187.86552 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11453.98885 HOMO: -7.01782 LUMO: -1.08846 factor:1 | 1 (-1.75764) | -1 | -1 |
| G: -5187.86552 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11454.13209 HOMO: -7.03959 LUMO: -1.15376 factor:1 | 1 (-1.90088) | -1 | -1 |
| G: -5187.86552 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11452.21282 HOMO: -6.68856 LUMO: 1.61364 factor:1 | -1 (0.01839) | -1 | -1 |
| G: -5187.86552 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11451.82939 HOMO: -6.53345 LUMO: 1.60275 factor:1 | -1 (0.40183) | -1 | -1 |
| G: -5187.86552 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11452.71542 HOMO: -6.73482 LUMO: 1.86398 factor:1 | 1 (-0.48420) | -1 | -1 |
| G: -5187.86552 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11452.72347 HOMO: -6.87632 LUMO: 1.59731 factor:1 | 1 (-0.49225) | -1 | -1 |
| G: -5187.86552 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11452.62262 HOMO: -6.31848 LUMO: 2.12521 factor:1 | 1 (-0.39141) | -1 | -1 |
| G: -5187.86552 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11452.77087 HOMO: -6.35114 LUMO: 1.71432 factor:1 | 1 (-0.53966) | -1 | -1 |
| G: -5187.86552 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11452.66491 HOMO: -6.34842 LUMO: 1.92929 factor:1 | 1 (-0.43370) | -1 | -1 |
| G: -5187.86552 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11451.49300 HOMO: -6.14977 LUMO: 1.78235 factor:1 | -1 (0.73822) | -1 | -1 |
| G: -5187.86552 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11451.71308 HOMO: -6.31032 LUMO: 1.51567 factor:1 | -1 (0.51813) | -1 | -1 |
| G: -5187.86552 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11451.96650 HOMO: -6.25862 LUMO: 1.75241 factor:1 | -1 (0.26471) | -1 | -1 |
| G: -5187.86552 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11452.32289 HOMO: -6.49264 LUMO: 1.66806 factor:1 | 1 (-0.09168) | -1 | -1 |
| G: -5187.86552 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11452.66497 HOMO: -6.28311 LUMO: 1.60003 factor:1 | 1 (-0.43375) | -1 | -1 |
| G: -5187.86552 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11453.59940 HOMO: -7.13210 LUMO: -0.04354 factor:1 | 1 (-1.36819) | 1 | 1 |
| G: -5187.86552 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11453.72869 HOMO: -7.35252 LUMO: 0.03537 factor:1 | 1 (-1.49747) | 1 | 1 |
| G: -5187.86552 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11452.98854 HOMO: -6.58243 LUMO: -0.48980 factor:1 | 1 (-0.75732) | -1 | -1 |
| G: -5187.86552 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11453.89633 HOMO: -6.90081 LUMO: -0.05442 factor:1 | 1 (-1.66512) | -1 | -1 |
| G: -5187.86552 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11453.77394 HOMO: -7.22734 LUMO: 0.17143 factor:1 | 1 (-1.54272) | 1 | 1 |
| G: -5187.86552 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11452.88611 HOMO: -7.13210 LUMO: -0.99866 factor:1 | 1 (-0.65490) | 1 | 1 |
| G: -5187.86552 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11454.04121 HOMO: -7.39878 LUMO: 0.13334 factor:1 | 1 (-1.80999) | 1 | 1 |
| G: -5187.86552 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11453.16029 HOMO: -7.04503 LUMO: -0.89798 factor:1 | 1 (-0.92908) | -1 | -1 |
| G: -5187.86552 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11453.07861 HOMO: -6.95523 LUMO: -1.07213 factor:1 | 1 (-0.84739) | -1 | -1 |
| G: -5187.86552 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11452.92992 HOMO: -6.75114 LUMO: -1.28438 factor:1 | 1 (-0.69871) | -1 | -1 |
| G: -5187.86552 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11453.71255 HOMO: -6.75114 LUMO: -0.11701 factor:1 | 1 (-1.48133) | -1 | -1 |
| G: -5187.86552 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11453.71750 HOMO: -6.83278 LUMO: -0.01633 factor:1 | 1 (-1.48629) | -1 | -1 |
| G: -5187.86552 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11453.22596 HOMO: -6.93890 LUMO: -0.88981 factor:1 | 1 (-0.99474) | -1 | -1 |
| G: -5187.86552 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11453.13722 HOMO: -7.07224 LUMO: -1.08573 factor:1 | 1 (-0.90600) | 1 | 1 |
| G: -5187.86552 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11452.61256 HOMO: -6.99877 LUMO: -0.95240 factor:1 | 1 (-0.38134) | -1 | -1 |
| G: -5187.86552 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11453.48503 HOMO: -7.09129 LUMO: 0.35375 factor:1 | 1 (-1.25382) | 1 | 1 |
| G: -5187.86552 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11453.34332 HOMO: -7.09401 LUMO: 0.04354 factor:1 | 1 (-1.11210) | 1 | 1 |
| G: -5187.86552 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11453.63364 HOMO: -6.85183 LUMO: -0.68573 factor:1 | 1 (-1.40242) | -1 | -1 |
| G: -5187.86552 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11453.72245 HOMO: -6.83006 LUMO: -0.58777 factor:1 | 1 (-1.49124) | -1 | -1 |
| G: -5187.86552 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11454.51991 HOMO: -7.40422 LUMO: 0.17687 factor:1 | 1 (-2.28870) | 1 | 1 |
| G: -5187.86552 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11454.18205 HOMO: -7.15932 LUMO: 0.10340 factor:1 | 1 (-1.95084) | 1 | 1 |
| G: -5187.86552 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11453.44936 HOMO: -7.03414 LUMO: -0.19592 factor:1 | 1 (-1.21814) | -1 | -1 |
| G: -5187.86552 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11452.90432 HOMO: -6.48447 LUMO: -0.36191 factor:1 | 1 (-0.67310) | -1 | -1 |
| G: -5187.86552 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11454.24668 HOMO: -7.49402 LUMO: 0.11429 factor:1 | 1 (-2.01547) | 1 | 1 |
| G: -5187.86552 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11453.30560 HOMO: -7.01237 LUMO: -1.06397 factor:1 | 1 (-1.07439) | -1 | -1 |
| G: -5187.86552 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11453.32389 HOMO: -6.67223 LUMO: -1.07213 factor:1 | 1 (-1.09267) | -1 | -1 |
| G: -5187.86552 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11453.14326 HOMO: -7.38789 LUMO: -1.15376 factor:1 | 1 (-0.91204) | 1 | 1 |
| G: -5187.86552 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11453.09368 HOMO: -6.42461 LUMO: -1.23812 factor:1 | 1 (-0.86246) | -1 | -1 |
| G: -5187.86552 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11453.29973 HOMO: -7.36884 LUMO: -1.19186 factor:1 | 1 (-1.06851) | 1 | 1 |
| G: -5187.86552 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11454.03650 HOMO: -6.65591 LUMO: 0.07075 factor:1 | 1 (-1.80528) | -1 | -1 |
| G: -5187.86552 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11453.86850 HOMO: -7.39061 LUMO: -0.16871 factor:1 | 1 (-1.63728) | 1 | 1 |
| G: -5187.86552 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11453.50958 HOMO: -6.90353 LUMO: -0.96056 factor:1 | 1 (-1.27836) | -1 | -1 |
| G: -5187.86552 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11453.53663 HOMO: -7.42054 LUMO: 0.19048 factor:1 | 1 (-1.30541) | 1 | 1 |
| G: -5187.86552 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11453.46776 HOMO: -7.40150 LUMO: 0.35647 factor:1 | 1 (-1.23654) | 1 | 1 |
| G: -5187.86552 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11452.61201 HOMO: -6.56067 LUMO: -0.96056 factor:1 | 1 (-0.38080) | -1 | -1 |
| G: -5187.86552 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11453.00048 HOMO: -6.89809 LUMO: -0.81090 factor:1 | 1 (-0.76927) | -1 | -1 |
| G: -5187.86552 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11453.21202 HOMO: -6.91986 LUMO: -0.84900 factor:1 | 1 (-0.98081) | -1 | -1 |
| G: -5187.86552 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11453.92806 HOMO: -6.61509 LUMO: -0.62042 factor:1 | 1 (-1.69685) | -1 | -1 |
| G: -5187.86552 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11453.90983 HOMO: -6.58243 LUMO: -0.65579 factor:1 | 1 (-1.67862) | -1 | -1 |
| G: -5187.86552 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11453.54770 HOMO: -6.52257 LUMO: -0.92519 factor:1 | 1 (-1.31649) | -1 | -1 |
| G: -5187.86552 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11452.06974 HOMO: -6.69128 LUMO: 1.49118 factor:1 | -1 (0.16147) | -1 | -1 |
| G: -5187.86552 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11451.98076 HOMO: -7.02870 LUMO: 1.67894 factor:1 | -1 (0.25045) | -1 | -1 |
| G: -5187.86552 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11452.67705 HOMO: -6.88720 LUMO: 1.68711 factor:1 | 1 (-0.44583) | -1 | -1 |
| G: -5187.86552 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11451.91047 HOMO: -5.89943 LUMO: 1.03675 factor:1 | -1 (0.32074) | -1 | -1 |
| G: -5187.86552 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11451.81687 HOMO: -6.40556 LUMO: 1.14560 factor:1 | -1 (0.41435) | -1 | -1 |
| G: -5187.86552 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11452.07407 HOMO: -6.51168 LUMO: 1.48030 factor:1 | -1 (0.15715) | -1 | -1 |
| G: -5187.86552 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11452.66309 HOMO: -6.64502 LUMO: 1.91568 factor:1 | 1 (-0.43187) | -1 | -1 |
| G: -5187.86552 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11452.59637 HOMO: -6.47903 LUMO: 1.91296 factor:1 | 1 (-0.36515) | -1 | -1 |
| G: -5187.86552 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11452.68529 HOMO: -6.34297 LUMO: 1.91840 factor:1 | 1 (-0.45408) | -1 | -1 |
| G: -5187.86552 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11451.25188 HOMO: -6.89809 LUMO: 1.82861 factor:1 | -1 (0.97934) | -1 | -1 |
| G: -5187.86552 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11451.73512 HOMO: -6.10079 LUMO: 1.62996 factor:1 | -1 (0.49609) | -1 | -1 |
| G: -5187.86552 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11454.41096 HOMO: -7.16476 LUMO: -0.92247 factor:1 | 1 (-2.17974) | 1 | 1 |
| G: -5187.86552 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11453.60517 HOMO: -7.10489 LUMO: -0.95784 factor:1 | 1 (-1.37396) | 1 | 1 |
| G: -5187.86552 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11452.67544 HOMO: -6.76475 LUMO: -0.99866 factor:1 | 1 (-0.44423) | -1 | -1 |
| G: -5187.86552 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11452.79996 HOMO: -6.81373 LUMO: -1.05036 factor:1 | 1 (-0.56875) | -1 | -1 |
| G: -5187.86552 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11452.88119 HOMO: -6.90081 LUMO: -1.03947 factor:1 | 1 (-0.64997) | -1 | -1 |
| G: -5187.86552 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11453.68507 HOMO: -7.06952 LUMO: -0.91702 factor:1 | 1 (-1.45385) | 1 | 1 |
| G: -5187.86552 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11453.45407 HOMO: -6.73482 LUMO: -0.94151 factor:1 | 1 (-1.22285) | -1 | -1 |
| G: -5187.86552 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11453.56332 HOMO: -6.99605 LUMO: -1.04764 factor:1 | 1 (-1.33211) | -1 | -1 |
| G: -5187.86552 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11453.61279 HOMO: -7.03686 LUMO: -0.93335 factor:1 | 1 (-1.38158) | -1 | -1 |
| G: -5187.86552 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11452.52997 HOMO: -6.81101 LUMO: -0.95240 factor:1 | 1 (-0.29875) | -1 | -1 |
| G: -5187.86552 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11452.75131 HOMO: -6.83822 LUMO: -0.65307 factor:1 | 1 (-0.52009) | -1 | -1 |
| G: -5187.86552 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11452.58534 HOMO: -7.05319 LUMO: -0.81634 factor:1 | 1 (-0.35413) | -1 | -1 |
| G: -5187.86552 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11453.43684 HOMO: -7.57565 LUMO: 0.19048 factor:1 | 1 (-1.20563) | 1 | 1 |
| G: -5187.86552 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11452.66009 HOMO: -6.56067 LUMO: -0.50613 factor:1 | 1 (-0.42888) | -1 | -1 |
| G: -5187.86552 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11452.98075 HOMO: -6.74298 LUMO: -0.70477 factor:1 | 1 (-0.74954) | -1 | -1 |
| G: -5187.86552 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11453.09224 HOMO: -7.02054 LUMO: 0.03537 factor:1 | 1 (-0.86102) | -1 | -1 |
| G: -5187.86552 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11453.44912 HOMO: -7.33347 LUMO: -0.17960 factor:1 | 1 (-1.21790) | 1 | 1 |
| G: -5187.86552 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11452.92026 HOMO: -6.98244 LUMO: -0.88165 factor:1 | 1 (-0.68905) | -1 | -1 |
| G: -5187.86552 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11452.63871 HOMO: -7.14843 LUMO: -1.19730 factor:1 | 1 (-0.40749) | 1 | 1 |
| G: -5187.86552 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11452.89882 HOMO: -7.17564 LUMO: -1.21907 factor:1 | 1 (-0.66760) | 1 | 1 |
| G: -5187.86552 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11453.62063 HOMO: -6.74026 LUMO: -0.86532 factor:1 | 1 (-1.38941) | -1 | -1 |
| G: -5187.86552 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11453.66648 HOMO: -6.82462 LUMO: -1.24084 factor:1 | 1 (-1.43526) | -1 | -1 |
| G: -5187.86552 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11453.57516 HOMO: -6.78924 LUMO: -0.70477 factor:1 | 1 (-1.34394) | -1 | -1 |
| G: -5187.86552 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11454.69379 HOMO: -7.41238 LUMO: 0.05987 factor:1 | 1 (-2.46258) | 1 | 1 |
| G: -5187.86552 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11454.37773 HOMO: -6.75931 LUMO: 0.02721 factor:1 | 1 (-2.14652) | -1 | -1 |
| G: -5187.86552 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11453.48718 HOMO: -6.28583 LUMO: -0.93063 factor:1 | 1 (-1.25597) | -1 | -1 |
| G: -5187.86552 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11453.84235 HOMO: -6.69128 LUMO: -0.83539 factor:1 | 1 (-1.61113) | -1 | -1 |
| G: -5187.86552 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11454.77913 HOMO: -7.22190 LUMO: 0.01361 factor:1 | 1 (-2.54791) | 1 | 1 |
| G: -5187.86552 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11453.87467 HOMO: -6.95251 LUMO: -1.09934 factor:1 | 1 (-1.64346) | -1 | -1 |
| G: -5187.86552 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11453.92308 HOMO: -6.75387 LUMO: -0.90614 factor:1 | 1 (-1.69187) | -1 | -1 |
| G: -5187.86552 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11453.48876 HOMO: -7.48585 LUMO: 0.05987 factor:1 | 1 (-1.25755) | 1 | 1 |
| G: -5187.86552 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11452.90492 HOMO: -6.92802 LUMO: -0.66940 factor:1 | 1 (-0.67370) | -1 | -1 |
| G: -5187.86552 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11453.80186 HOMO: -7.29537 LUMO: -0.14150 factor:1 | 1 (-1.57064) | 1 | 1 |
| G: -5187.86552 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11452.72483 HOMO: -6.57155 LUMO: -0.86804 factor:1 | 1 (-0.49361) | -1 | -1 |
| G: -5187.86552 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11453.08516 HOMO: -6.87632 LUMO: -0.77825 factor:1 | 1 (-0.85395) | -1 | -1 |
| G: -5187.86552 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11453.06095 HOMO: -6.45998 LUMO: -0.31565 factor:1 | 1 (-0.82973) | -1 | -1 |
| G: -5187.86552 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11454.23708 HOMO: -7.51306 LUMO: 0.05714 factor:1 | 1 (-2.00586) | 1 | 1 |
| G: -5187.86552 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11453.96385 HOMO: -6.86271 LUMO: -0.00816 factor:1 | 1 (-1.73263) | -1 | -1 |
| G: -5187.86552 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11453.10919 HOMO: -6.43277 LUMO: -1.07485 factor:1 | 1 (-0.87798) | -1 | -1 |
| G: -5187.86552 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11453.38139 HOMO: -6.78108 LUMO: -0.81362 factor:1 | 1 (-1.15017) | -1 | -1 |
| G: -5187.86552 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11451.98479 HOMO: -6.88448 LUMO: 1.21907 factor:1 | -1 (0.24643) | -1 | -1 |
| G: -5187.86552 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11451.99668 HOMO: -6.97700 LUMO: 1.44765 factor:1 | -1 (0.23453) | -1 | -1 |
| G: -5187.86552 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11452.65713 HOMO: -6.89537 LUMO: 2.12249 factor:1 | 1 (-0.42591) | -1 | -1 |
| G: -5187.86552 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11451.49534 HOMO: -6.28311 LUMO: 1.45037 factor:1 | -1 (0.73588) | -1 | -1 |
| G: -5187.86552 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11451.76508 HOMO: -6.55522 LUMO: 1.39867 factor:1 | -1 (0.46613) | -1 | -1 |
| G: -5187.86552 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11451.82762 HOMO: -6.46815 LUMO: 1.50207 factor:1 | -1 (0.40360) | -1 | -1 |
| G: -5187.86552 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11452.54643 HOMO: -6.43549 LUMO: 2.17419 factor:1 | 1 (-0.31522) | -1 | -1 |
| G: -5187.86552 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11452.79648 HOMO: -6.99333 LUMO: 1.87214 factor:1 | 1 (-0.56526) | -1 | -1 |
| G: -5187.86552 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11452.63228 HOMO: -6.65591 LUMO: 1.37962 factor:1 | 1 (-0.40107) | -1 | -1 |
| G: -5187.86552 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11452.17309 HOMO: -6.82734 LUMO: 1.55649 factor:1 | -1 (0.05812) | -1 | -1 |
| G: -5187.86552 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11452.24817 HOMO: -6.71849 LUMO: 1.36057 factor:1 | 1 (-0.01695) | -1 | -1 |
| G: -5187.86552 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11452.62842 HOMO: -6.79468 LUMO: 1.82044 factor:1 | 1 (-0.39720) | -1 | -1 |
| G: -5187.86552 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11452.07358 HOMO: -6.61237 LUMO: 1.15104 factor:1 | -1 (0.15764) | -1 | -1 |
| G: -5187.86552 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11453.40838 HOMO: -6.62053 LUMO: 2.33474 factor:1 | 1 (-1.17716) | -1 | -1 |
| G: -5187.86552 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11452.15364 HOMO: -6.55794 LUMO: 1.65717 factor:1 | -1 (0.07758) | -1 | -1 |
| G: -5187.86552 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11453.16723 HOMO: -6.85999 LUMO: 2.03813 factor:1 | 1 (-0.93602) | -1 | -1 |
| G: -5187.86552 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11452.64575 HOMO: -6.45726 LUMO: 1.28438 factor:1 | 1 (-0.41454) | -1 | -1 |
| G: -5187.86552 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11452.55109 HOMO: -6.23685 LUMO: 1.93201 factor:1 | 1 (-0.31987) | -1 | -1 |
| G: -5187.86552 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11453.01409 HOMO: -7.06680 LUMO: 1.86942 factor:1 | 1 (-0.78287) | 1 | 1 |
| G: -5187.86552 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11453.54672 HOMO: -6.89537 LUMO: 2.17147 factor:1 | 1 (-1.31551) | -1 | -1 |
| G: -5187.86552 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11453.45151 HOMO: -6.80013 LUMO: 1.78779 factor:1 | 1 (-1.22029) | -1 | -1 |
| G: -5187.86552 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11450.84169 HOMO: -6.45726 LUMO: 1.58370 factor:1 | -1 (1.38952) | -1 | -1 |
| G: -5187.86552 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11451.05552 HOMO: -6.52529 LUMO: 1.71976 factor:1 | -1 (1.17570) | -1 | -1 |
| G: -5187.86552 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11453.19423 HOMO: -7.22462 LUMO: -1.18642 factor:1 | 1 (-0.96301) | 1 | 1 |
| G: -5187.86552 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11453.33181 HOMO: -7.18381 LUMO: -0.78641 factor:1 | 1 (-1.10059) | 1 | 1 |
| G: -5187.86552 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11451.93156 HOMO: -6.93346 LUMO: 1.65717 factor:1 | -1 (0.29965) | -1 | -1 |
| G: -5187.86552 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11452.11263 HOMO: -6.41644 LUMO: 1.78235 factor:1 | -1 (0.11859) | -1 | -1 |
| G: -5187.86552 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11452.45653 HOMO: -6.59876 LUMO: 1.83677 factor:1 | 1 (-0.22531) | -1 | -1 |
| G: -5187.86552 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11452.56975 HOMO: -6.35658 LUMO: 1.59731 factor:1 | 1 (-0.33854) | -1 | -1 |
| G: -5187.86552 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11453.08524 HOMO: -6.60692 LUMO: 1.66534 factor:1 | 1 (-0.85403) | -1 | -1 |
| G: -5187.86552 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11453.39608 HOMO: -6.83006 LUMO: 2.11705 factor:1 | 1 (-1.16487) | -1 | -1 |
| G: -5187.86552 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11451.94650 HOMO: -6.89264 LUMO: 1.30070 factor:1 | -1 (0.28471) | -1 | -1 |
| G: -5187.86552 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11452.68034 HOMO: -6.90081 LUMO: 2.05174 factor:1 | 1 (-0.44912) | -1 | -1 |
| G: -5187.86552 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11453.39965 HOMO: -6.74842 LUMO: 1.96194 factor:1 | 1 (-1.16843) | -1 | -1 |
| G: -5187.86552 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11451.78451 HOMO: -6.58516 LUMO: 1.30887 factor:1 | -1 (0.44670) | -1 | -1 |
| G: -5187.86552 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11452.63620 HOMO: -7.00965 LUMO: 2.08167 factor:1 | 1 (-0.40499) | -1 | -1 |
| G: -5187.86552 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11452.77193 HOMO: -6.86815 LUMO: 2.29664 factor:1 | 1 (-0.54072) | -1 | -1 |
| G: -5187.86552 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11452.66589 HOMO: -6.39740 LUMO: 2.02725 factor:1 | 1 (-0.43467) | -1 | -1 |
| G: -5187.86552 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11452.25318 HOMO: -5.95929 LUMO: 1.62724 factor:1 | 1 (-0.02196) | -1 | -1 |
| G: -5187.86552 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11452.67307 HOMO: -6.71849 LUMO: 1.34696 factor:1 | 1 (-0.44186) | -1 | -1 |
| G: -5187.86552 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11452.54836 HOMO: -7.26816 LUMO: 1.74153 factor:1 | 1 (-0.31715) | 1 | 1 |
| G: -5187.86552 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11452.96606 HOMO: -6.90897 LUMO: 1.71432 factor:1 | 1 (-0.73484) | -1 | -1 |
| G: -5187.86552 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11452.72282 HOMO: -6.70489 LUMO: 1.91568 factor:1 | 1 (-0.49160) | -1 | -1 |
| G: -5187.86552 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11452.72687 HOMO: -6.83278 LUMO: 1.61908 factor:1 | 1 (-0.49566) | -1 | -1 |
| G: -5187.86552 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11451.99331 HOMO: -7.17292 LUMO: 1.95378 factor:1 | -1 (0.23791) | 1 | -1 |
| G: -5187.86552 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11451.66867 HOMO: -6.53345 LUMO: 1.74153 factor:1 | -1 (0.56254) | -1 | -1 |
| G: -5187.86552 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11452.45345 HOMO: -6.53073 LUMO: 1.51023 factor:1 | 1 (-0.22224) | -1 | -1 |
| G: -5187.86552 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11453.32217 HOMO: -6.93346 LUMO: 2.22861 factor:1 | 1 (-1.09096) | -1 | -1 |
| G: -5187.86552 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11451.82269 HOMO: -6.47903 LUMO: 2.05446 factor:1 | -1 (0.40852) | -1 | -1 |
| G: -5187.86552 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11452.06231 HOMO: -6.88992 LUMO: 1.57010 factor:1 | -1 (0.16890) | -1 | -1 |
| G: -5187.86552 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11452.07913 HOMO: -6.07358 LUMO: 1.95922 factor:1 | -1 (0.15208) | -1 | -1 |
| G: -5187.86552 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11452.42624 HOMO: -6.75114 LUMO: 2.18780 factor:1 | 1 (-0.19502) | -1 | -1 |
| G: -5187.86552 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11452.09744 HOMO: -6.96339 LUMO: 1.70071 factor:1 | -1 (0.13377) | -1 | -1 |
| G: -5187.86552 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11451.92114 HOMO: -7.14843 LUMO: 1.82588 factor:1 | -1 (0.31007) | 1 | -1 |
| G: -5187.86552 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11452.61196 HOMO: -6.96339 LUMO: 2.29392 factor:1 | 1 (-0.38074) | -1 | -1 |
| G: -5187.86552 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11452.62877 HOMO: -6.81645 LUMO: 2.39732 factor:1 | 1 (-0.39756) | -1 | -1 |
| G: -5187.86552 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11451.82672 HOMO: -6.48447 LUMO: 1.24084 factor:1 | -1 (0.40450) | -1 | -1 |
| G: -5187.86552 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11451.96857 HOMO: -7.14843 LUMO: 2.01092 factor:1 | -1 (0.26264) | 1 | -1 |
| G: -5625.88943 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11890.04669 HOMO: -7.20013 LUMO: -0.34286 factor:1 | -1 (0.20844) | 1 | -1 |
| G: -5625.88943 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11889.06749 HOMO: -6.97700 LUMO: -0.15238 factor:1 | -1 (1.18764) | -1 | -1 |
| G: -5625.88943 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11889.15900 HOMO: -7.07768 LUMO: -0.26123 factor:1 | -1 (1.09613) | 1 | -1 |
| G: -5625.88943 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11888.71205 HOMO: -6.99333 LUMO: -0.41361 factor:1 | -1 (1.54308) | -1 | -1 |
| G: -5625.88943 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11888.63039 HOMO: -6.84638 LUMO: -0.40273 factor:1 | -1 (1.62474) | -1 | -1 |
| G: -5625.88943 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11888.41420 HOMO: -6.83822 LUMO: -0.26939 factor:1 | -1 (1.84093) | -1 | -1 |
| G: -5625.88943 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11891.61439 HOMO: -6.75931 LUMO: -0.93879 factor:1 | 1 (-1.35926) | -1 | -1 |
| G: -5625.88943 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11892.31704 HOMO: -6.79468 LUMO: -0.39729 factor:1 | 1 (-2.06192) | -1 | -1 |
| G: -5625.88943 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11892.47343 HOMO: -6.93890 LUMO: 0.43266 factor:1 | 1 (-2.21830) | -1 | -1 |
| G: -5625.88943 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11892.12431 HOMO: -7.08040 LUMO: -0.85716 factor:1 | 1 (-1.86918) | 1 | 1 |
| G: -5625.88943 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11891.73586 HOMO: -6.70216 LUMO: -1.41499 factor:1 | 1 (-1.48073) | -1 | -1 |
| G: -5625.88943 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11891.81976 HOMO: -6.63686 LUMO: -0.52790 factor:1 | 1 (-1.56463) | -1 | -1 |
| G: -5625.88943 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11892.51250 HOMO: -6.75114 LUMO: -0.13334 factor:1 | 1 (-2.25737) | -1 | -1 |
| G: -5625.88943 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11892.53759 HOMO: -6.94435 LUMO: -0.24490 factor:1 | 1 (-2.28246) | -1 | -1 |
| G: -5625.88943 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11891.71959 HOMO: -6.74298 LUMO: -0.84627 factor:1 | 1 (-1.46446) | -1 | -1 |
| G: -5625.88943 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11892.15007 HOMO: -7.15932 LUMO: 0.22041 factor:1 | 1 (-1.89495) | 1 | 1 |
| G: -5625.88943 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11891.27019 HOMO: -6.90081 LUMO: -1.16737 factor:1 | 1 (-1.01507) | -1 | -1 |
| G: -5625.88943 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11892.00509 HOMO: -7.04775 LUMO: -0.84355 factor:1 | 1 (-1.74996) | -1 | -1 |
| G: -5625.88943 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11891.32511 HOMO: -7.17020 LUMO: -1.31159 factor:1 | 1 (-1.06998) | 1 | 1 |
| G: -5625.88943 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11892.36107 HOMO: -7.14571 LUMO: -0.46259 factor:1 | 1 (-2.10594) | 1 | 1 |
| G: -5625.88943 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11890.70779 HOMO: -7.45048 LUMO: -0.91158 factor:1 | 1 (-0.45266) | 1 | 1 |
| G: -5625.88943 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11891.28723 HOMO: -6.87360 LUMO: -0.82995 factor:1 | 1 (-1.03210) | -1 | -1 |
| G: -5625.88943 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11890.90129 HOMO: -7.43415 LUMO: -0.65307 factor:1 | 1 (-0.64616) | 1 | 1 |
| G: -5625.88943 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11891.06097 HOMO: -7.47225 LUMO: -0.77280 factor:1 | 1 (-0.80584) | 1 | 1 |
| G: -5625.88943 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11891.72169 HOMO: -6.86271 LUMO: -0.83811 factor:1 | 1 (-1.46656) | -1 | -1 |
| G: -5625.88943 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11891.28492 HOMO: -7.53483 LUMO: -0.66124 factor:1 | 1 (-1.02979) | 1 | 1 |
| G: -5625.88943 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11891.22758 HOMO: -7.45864 LUMO: -1.08301 factor:1 | 1 (-0.97245) | 1 | 1 |
| G: -5625.88943 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11891.88623 HOMO: -7.24639 LUMO: -1.19186 factor:1 | 1 (-1.63110) | 1 | 1 |
| G: -5625.88943 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11891.42941 HOMO: -7.54844 LUMO: -0.96873 factor:1 | 1 (-1.17428) | 1 | 1 |
| G: -5625.88943 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11892.04286 HOMO: -7.12666 LUMO: -0.01633 factor:1 | 1 (-1.78773) | 1 | 1 |
| G: -5625.88943 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11891.68030 HOMO: -6.77291 LUMO: -0.70477 factor:1 | 1 (-1.42517) | -1 | -1 |
| G: -5625.88943 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11892.40529 HOMO: -6.76475 LUMO: -1.15921 factor:1 | 1 (-2.15016) | -1 | -1 |
| G: -5625.88943 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11890.11121 HOMO: -5.37697 LUMO: -0.56600 factor:1 | -1 (0.14392) | -1 | -1 |
| G: -5625.88943 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11891.40930 HOMO: -6.62053 LUMO: -1.75513 factor:1 | 1 (-1.15417) | -1 | -1 |
| G: -5625.88943 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11891.76571 HOMO: -6.60420 LUMO: -1.74697 factor:1 | 1 (-1.51059) | -1 | -1 |
| G: -5625.88943 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11892.16741 HOMO: -6.84366 LUMO: -0.94968 factor:1 | 1 (-1.91228) | -1 | -1 |
| G: -5625.88943 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11891.91295 HOMO: -6.96884 LUMO: -2.11977 factor:1 | 1 (-1.65783) | -1 | -1 |
| G: -5625.88943 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11890.68768 HOMO: -6.80829 LUMO: 0.56055 factor:1 | 1 (-0.43255) | -1 | -1 |
| G: -5625.88943 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11890.61054 HOMO: -7.02326 LUMO: 0.11429 factor:1 | 1 (-0.35541) | -1 | -1 |
| G: -5625.88943 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11890.84880 HOMO: -7.40966 LUMO: 0.18232 factor:1 | 1 (-0.59367) | 1 | 1 |
| G: -5625.88943 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11890.94646 HOMO: -6.34570 LUMO: 0.41089 factor:1 | 1 (-0.69133) | -1 | -1 |
| G: -5625.88943 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11890.93373 HOMO: -6.78924 LUMO: 0.49525 factor:1 | 1 (-0.67860) | -1 | -1 |
| G: -5625.88943 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11890.99849 HOMO: -6.87632 LUMO: 0.44082 factor:1 | 1 (-0.74336) | -1 | -1 |
| G: -5625.88943 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11890.97549 HOMO: -6.69944 LUMO: 1.20546 factor:1 | 1 (-0.72037) | -1 | -1 |
| G: -5625.88943 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11891.01462 HOMO: -6.83006 LUMO: 1.28982 factor:1 | 1 (-0.75950) | -1 | -1 |
| G: -5625.88943 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11890.50085 HOMO: -7.78246 LUMO: 0.20681 factor:1 | 1 (-0.24572) | 1 | 1 |
| G: -5625.88943 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11891.54266 HOMO: -6.55794 LUMO: -1.65173 factor:1 | 1 (-1.28753) | -1 | -1 |
| G: -5625.88943 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11892.17149 HOMO: -6.77564 LUMO: -1.14560 factor:1 | 1 (-1.91636) | -1 | -1 |
| G: -5625.88943 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11891.83488 HOMO: -7.46680 LUMO: -1.18097 factor:1 | 1 (-1.57976) | 1 | 1 |
| G: -5625.88943 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11891.67322 HOMO: -6.88176 LUMO: -1.24900 factor:1 | 1 (-1.41809) | -1 | -1 |
| G: -5625.88943 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11892.31895 HOMO: -7.28177 LUMO: -0.42178 factor:1 | 1 (-2.06382) | 1 | 1 |
| G: -5625.88943 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11890.32460 HOMO: -7.71715 LUMO: 0.19592 factor:1 | 1 (-0.06947) | 1 | 1 |
| G: -5625.88943 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11891.38421 HOMO: -7.02326 LUMO: -1.40683 factor:1 | 1 (-1.12908) | -1 | -1 |
| G: -5625.88943 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11890.58267 HOMO: -7.27088 LUMO: -1.07485 factor:1 | 1 (-0.32754) | 1 | 1 |
| G: -5625.88943 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11891.03286 HOMO: -7.17020 LUMO: -0.49525 factor:1 | 1 (-0.77773) | 1 | 1 |
| G: -5625.88943 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11891.84460 HOMO: -7.15932 LUMO: 0.02721 factor:1 | 1 (-1.58947) | 1 | 1 |
| G: -5625.88943 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11891.84846 HOMO: -7.00693 LUMO: -0.83267 factor:1 | 1 (-1.59334) | -1 | -1 |
| G: -5625.88943 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11892.17348 HOMO: -6.86543 LUMO: -0.10340 factor:1 | 1 (-1.91835) | -1 | -1 |
| G: -5625.88943 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11891.11220 HOMO: -7.11850 LUMO: -0.08980 factor:1 | 1 (-0.85708) | 1 | 1 |
| G: -5625.88943 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11891.83031 HOMO: -6.87087 LUMO: -0.88981 factor:1 | 1 (-1.57519) | -1 | -1 |
| G: -5625.88943 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11891.61583 HOMO: -7.08857 LUMO: -1.27077 factor:1 | 1 (-1.36071) | 1 | 1 |
| G: -5625.88943 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11890.28574 HOMO: -6.79468 LUMO: -0.81906 factor:1 | 1 (-0.03061) | -1 | -1 |
| G: -5625.88943 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11891.40614 HOMO: -6.86815 LUMO: -0.89798 factor:1 | 1 (-1.15101) | -1 | -1 |
| G: -5625.88943 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11891.37194 HOMO: -6.78652 LUMO: -2.00548 factor:1 | 1 (-1.11681) | -1 | -1 |
| G: -5625.88943 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11890.78529 HOMO: -6.75114 LUMO: -0.08436 factor:1 | 1 (-0.53016) | -1 | -1 |
| G: -5625.88943 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11890.80918 HOMO: -6.55794 LUMO: 0.52790 factor:1 | 1 (-0.55405) | -1 | -1 |
| G: -5625.88943 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11890.17200 HOMO: -7.17836 LUMO: 0.28300 factor:1 | -1 (0.08313) | 1 | -1 |
| G: -5625.88943 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11890.87606 HOMO: -7.35796 LUMO: -0.77552 factor:1 | 1 (-0.62094) | 1 | 1 |
| G: -5625.88943 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11891.28813 HOMO: -7.23551 LUMO: -1.17553 factor:1 | 1 (-1.03300) | 1 | 1 |
| G: -5625.88943 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11890.30887 HOMO: -7.07496 LUMO: -1.14288 factor:1 | 1 (-0.05374) | 1 | 1 |
| G: -5625.88943 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11891.31131 HOMO: -6.70489 LUMO: -0.83539 factor:1 | 1 (-1.05618) | -1 | -1 |
| G: -5625.88943 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11891.30179 HOMO: -6.59604 LUMO: -0.89798 factor:1 | 1 (-1.04666) | -1 | -1 |
| G: -5625.88943 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11891.53531 HOMO: -6.94162 LUMO: -1.22451 factor:1 | 1 (-1.28019) | -1 | -1 |
| G: -5625.88943 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11890.63407 HOMO: -6.68040 LUMO: 0.22041 factor:1 | 1 (-0.37895) | -1 | -1 |
| G: -5625.88943 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11890.69685 HOMO: -6.88176 LUMO: 0.11157 factor:1 | 1 (-0.44172) | -1 | -1 |
| G: -5625.88943 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11891.61874 HOMO: -6.91713 LUMO: 1.27621 factor:1 | 1 (-1.36362) | -1 | -1 |
| G: -5625.88943 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11890.57399 HOMO: -6.77836 LUMO: 1.01226 factor:1 | 1 (-0.31886) | -1 | -1 |
| G: -5625.88943 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11891.80397 HOMO: -7.14571 LUMO: 1.48574 factor:1 | 1 (-1.54884) | 1 | 1 |
| G: -5625.88943 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11890.92450 HOMO: -6.96884 LUMO: 1.48574 factor:1 | 1 (-0.66937) | -1 | -1 |
| G: -5625.88943 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11891.78903 HOMO: -7.24367 LUMO: 1.28438 factor:1 | 1 (-1.53391) | 1 | 1 |
| G: -5625.88943 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11890.90319 HOMO: -7.10489 LUMO: 1.29526 factor:1 | 1 (-0.64807) | 1 | 1 |
| G: -5625.88943 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11891.71763 HOMO: -7.07224 LUMO: 1.29254 factor:1 | 1 (-1.46250) | 1 | 1 |
| G: -5625.88943 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11890.67348 HOMO: -7.12938 LUMO: 0.49253 factor:1 | 1 (-0.41835) | 1 | 1 |
| G: -5625.88943 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11891.00608 HOMO: -7.33619 LUMO: 1.45581 factor:1 | 1 (-0.75095) | 1 | 1 |
| G: -5625.88943 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11890.76292 HOMO: -6.87904 LUMO: -0.14422 factor:1 | 1 (-0.50779) | -1 | -1 |
| G: -5625.88943 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11890.65601 HOMO: -6.81917 LUMO: 0.50341 factor:1 | 1 (-0.40088) | -1 | -1 |
| G: -5625.88943 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11890.07768 HOMO: -7.27905 LUMO: 0.13606 factor:1 | -1 (0.17745) | 1 | -1 |
| G: -5625.88943 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11891.11457 HOMO: -6.87904 LUMO: -0.09796 factor:1 | 1 (-0.85944) | -1 | -1 |
| G: -5625.88943 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11890.61339 HOMO: -7.33891 LUMO: 0.03810 factor:1 | 1 (-0.35827) | 1 | 1 |
| G: -5625.88943 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11890.35461 HOMO: -6.98516 LUMO: 0.98233 factor:1 | 1 (-0.09948) | -1 | -1 |
| G: -5625.88943 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11891.46533 HOMO: -6.94162 LUMO: 0.86804 factor:1 | 1 (-1.21020) | -1 | -1 |
| G: -5625.88943 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11891.47610 HOMO: -7.37701 LUMO: 0.05442 factor:1 | 1 (-1.22097) | 1 | 1 |
| G: -5625.88943 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11891.59273 HOMO: -7.04775 LUMO: 0.43266 factor:1 | 1 (-1.33760) | -1 | -1 |
| G: -5625.88943 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11890.88175 HOMO: -7.47497 LUMO: 0.31837 factor:1 | 1 (-0.62662) | 1 | 1 |
| G: -5625.88943 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11890.41812 HOMO: -6.62053 LUMO: 0.13061 factor:1 | 1 (-0.16300) | -1 | -1 |
| G: -5625.88943 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11889.50360 HOMO: -6.44366 LUMO: -0.04354 factor:1 | -1 (0.75152) | -1 | -1 |
| G: -5625.88943 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11890.47282 HOMO: -6.40284 LUMO: 0.68301 factor:1 | 1 (-0.21769) | -1 | -1 |
| G: -5625.88943 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11890.52308 HOMO: -6.73754 LUMO: 0.36735 factor:1 | 1 (-0.26795) | -1 | -1 |
| G: -5625.88943 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11890.76695 HOMO: -6.85455 LUMO: 0.23946 factor:1 | 1 (-0.51182) | -1 | -1 |
| G: -5625.88943 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11890.62599 HOMO: -6.93346 LUMO: 0.24762 factor:1 | 1 (-0.37086) | -1 | -1 |
| G: -5625.88943 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11890.70134 HOMO: -6.85455 LUMO: 0.17687 factor:1 | 1 (-0.44621) | -1 | -1 |
| G: -5625.88943 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11891.33496 HOMO: -6.62325 LUMO: 0.69933 factor:1 | 1 (-1.07983) | -1 | -1 |
| G: -5625.88943 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11891.23417 HOMO: -6.43005 LUMO: 0.50069 factor:1 | 1 (-0.97904) | -1 | -1 |
| G: -5625.88943 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11890.85827 HOMO: -6.56883 LUMO: 0.22858 factor:1 | 1 (-0.60314) | -1 | -1 |
| G: -5625.88943 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11890.80376 HOMO: -6.78380 LUMO: 0.54967 factor:1 | 1 (-0.54864) | -1 | -1 |
| G: -5625.88943 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11890.87419 HOMO: -7.35524 LUMO: 0.00272 factor:1 | 1 (-0.61906) | 1 | 1 |
| G: -5625.88943 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11891.80022 HOMO: -7.27360 LUMO: 0.08436 factor:1 | 1 (-1.54509) | 1 | 1 |
| G: -5625.88943 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11890.89710 HOMO: -7.44504 LUMO: -0.96056 factor:1 | 1 (-0.64197) | 1 | 1 |
| G: -5625.88943 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11890.59946 HOMO: -7.27360 LUMO: 0.29933 factor:1 | 1 (-0.34433) | 1 | 1 |
| G: -5625.88943 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11890.63826 HOMO: -7.09129 LUMO: 0.41089 factor:1 | 1 (-0.38314) | 1 | 1 |
| G: -5625.88943 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11890.67323 HOMO: -6.93618 LUMO: 0.36463 factor:1 | 1 (-0.41810) | -1 | -1 |
| G: -6199.43603 HOMO: -7.26000 LUMO: -3.02863 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -6232.52541 HOMO: -7.65728 LUMO: 0.20136 factor:2 | 1 (-1.24908) | 1 | 1 |
| G: -6199.43603 HOMO: -7.26000 LUMO: -3.02863 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -6231.94940 HOMO: -6.90353 LUMO: -0.92791 factor:2 | 1 (-0.09706) | -1 | -1 |
| G: -6199.43603 HOMO: -7.26000 LUMO: -3.02863 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12463.94225 HOMO: -6.82462 LUMO: -1.18370 factor:1 | 1 (-0.14052) | -1 | -1 |
| G: -6199.43603 HOMO: -7.26000 LUMO: -3.02863 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12464.76760 HOMO: -7.09129 LUMO: -0.13334 factor:1 | 1 (-0.96587) | 1 | 1 |
| G: -6199.43603 HOMO: -7.26000 LUMO: -3.02863 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12464.14312 HOMO: -7.40966 LUMO: -1.06941 factor:1 | 1 (-0.34139) | 1 | 1 |
| G: -6199.43603 HOMO: -7.26000 LUMO: -3.02863 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12463.98590 HOMO: -7.24367 LUMO: -1.00954 factor:1 | 1 (-0.18417) | 1 | 1 |
| G: -6199.43603 HOMO: -7.26000 LUMO: -3.02863 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12464.28563 HOMO: -7.51851 LUMO: 0.09796 factor:1 | 1 (-0.48390) | 1 | 1 |
| G: -6199.43603 HOMO: -7.26000 LUMO: -3.02863 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12464.71383 HOMO: -7.48857 LUMO: -0.07619 factor:1 | 1 (-0.91210) | 1 | 1 |
| G: -6199.43603 HOMO: -7.26000 LUMO: -3.02863 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12462.88593 HOMO: -6.53345 LUMO: 1.09390 factor:1 | -1 (0.91580) | -1 | -1 |
| G: -6199.43603 HOMO: -7.26000 LUMO: -3.02863 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12464.25447 HOMO: -7.21918 LUMO: 0.08436 factor:1 | 1 (-0.45274) | 1 | 1 |
| G: -6199.43603 HOMO: -7.26000 LUMO: -3.02863 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12463.50616 HOMO: -7.38789 LUMO: 1.02587 factor:1 | -1 (0.29557) | 1 | -1 |
| G: -4243.27934 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10509.35160 HOMO: -6.83550 LUMO: -0.67484 factor:1 | 1 (-1.70656) | -1 | -1 |
| G: -4243.27934 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10509.92018 HOMO: -7.04231 LUMO: 0.54151 factor:1 | 1 (-2.27514) | -1 | -1 |
| G: -4243.27934 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10508.27291 HOMO: -6.79740 LUMO: 1.91296 factor:1 | 1 (-0.62788) | 1 | 1 |
| G: -4243.27934 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10508.85801 HOMO: -7.35796 LUMO: -1.04220 factor:1 | 1 (-1.21297) | -1 | -1 |
| G: -4243.27934 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10508.82686 HOMO: -6.62597 LUMO: -0.44082 factor:1 | 1 (-1.18182) | -1 | -1 |
| G: -4243.27934 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10508.75926 HOMO: -6.45182 LUMO: -0.20409 factor:1 | 1 (-1.11422) | -1 | -1 |
| G: -4243.27934 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10509.24458 HOMO: -6.51168 LUMO: -0.23130 factor:1 | 1 (-1.59954) | -1 | -1 |
| G: -4243.27934 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10509.66951 HOMO: -7.14027 LUMO: 0.49797 factor:1 | 1 (-2.02447) | -1 | -1 |
| G: -4243.27934 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10509.34210 HOMO: -7.55660 LUMO: 0.24762 factor:1 | 1 (-1.69707) | -1 | -1 |
| G: -4243.27934 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10508.64726 HOMO: -6.88992 LUMO: -0.64763 factor:1 | 1 (-1.00222) | -1 | -1 |
| G: -4243.27934 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10508.88912 HOMO: -6.72665 LUMO: -0.45987 factor:1 | 1 (-1.24408) | -1 | -1 |
| G: -4243.27934 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10508.62805 HOMO: -6.72121 LUMO: -0.58232 factor:1 | 1 (-0.98301) | -1 | -1 |
| G: -4243.27934 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10509.37198 HOMO: -7.26816 LUMO: 0.32926 factor:1 | 1 (-1.72694) | -1 | -1 |
| G: -4243.27934 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10508.82977 HOMO: -6.57155 LUMO: -0.53606 factor:1 | 1 (-1.18473) | -1 | -1 |
| G: -4243.27934 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10508.52672 HOMO: -6.50896 LUMO: -0.43810 factor:1 | 1 (-0.88168) | -1 | -1 |
| G: -4243.27934 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10508.63123 HOMO: -6.73210 LUMO: -0.51430 factor:1 | 1 (-0.98620) | -1 | -1 |
| G: -4243.27934 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10508.84473 HOMO: -6.77019 LUMO: -0.62858 factor:1 | 1 (-1.19970) | -1 | -1 |
| G: -4243.27934 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10508.74745 HOMO: -6.82462 LUMO: -0.67484 factor:1 | 1 (-1.10241) | -1 | -1 |
| G: -4243.27934 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10508.52998 HOMO: -6.79740 LUMO: -0.55511 factor:1 | 1 (-0.88494) | -1 | -1 |
| G: -4243.27934 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10508.81856 HOMO: -6.79740 LUMO: -0.67756 factor:1 | 1 (-1.17352) | -1 | -1 |
| G: -4243.27934 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10508.78909 HOMO: -6.75114 LUMO: -0.55239 factor:1 | 1 (-1.14405) | -1 | -1 |
| G: -4243.27934 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10508.96248 HOMO: -6.49536 LUMO: -0.25307 factor:1 | 1 (-1.31744) | -1 | -1 |
| G: -4243.27934 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10509.17459 HOMO: -6.48992 LUMO: -0.25034 factor:1 | 1 (-1.52955) | -1 | -1 |
| G: -4243.27934 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10508.85611 HOMO: -6.52801 LUMO: -0.28028 factor:1 | 1 (-1.21107) | -1 | -1 |
| G: -4243.27934 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10509.83874 HOMO: -7.22462 LUMO: 0.52518 factor:1 | 1 (-2.19370) | -1 | -1 |
| G: -4243.27934 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10508.98289 HOMO: -6.59332 LUMO: -0.27211 factor:1 | 1 (-1.33785) | -1 | -1 |
| G: -4243.27934 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10509.21446 HOMO: -6.57427 LUMO: -0.16871 factor:1 | 1 (-1.56942) | -1 | -1 |
| G: -4243.27934 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10508.10339 HOMO: -6.71033 LUMO: 1.59187 factor:1 | 1 (-0.45835) | 1 | 1 |
| G: -4243.27934 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10508.12535 HOMO: -6.72121 LUMO: 2.00004 factor:1 | 1 (-0.48031) | 1 | 1 |
| G: -4243.27934 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10508.24679 HOMO: -6.61509 LUMO: 1.55921 factor:1 | 1 (-0.60175) | -1 | -1 |
| G: -4243.27934 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10508.24279 HOMO: -6.55250 LUMO: 1.73064 factor:1 | 1 (-0.59775) | -1 | -1 |
| G: -4243.27934 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10508.17297 HOMO: -6.66135 LUMO: 2.02181 factor:1 | 1 (-0.52793) | 1 | 1 |
| G: -4243.27934 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10507.96594 HOMO: -6.84911 LUMO: 1.98099 factor:1 | 1 (-0.32090) | 1 | 1 |
| G: -4243.27934 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10507.86738 HOMO: -6.66679 LUMO: 1.98371 factor:1 | 1 (-0.22234) | 1 | 1 |
| G: -4243.27934 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10507.98303 HOMO: -6.67495 LUMO: 2.04085 factor:1 | 1 (-0.33799) | 1 | 1 |
| G: -4243.27934 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10508.13147 HOMO: -6.89809 LUMO: 1.95106 factor:1 | 1 (-0.48643) | 1 | 1 |
| G: -4243.27934 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10508.69880 HOMO: -6.50352 LUMO: 1.88847 factor:1 | 1 (-1.05376) | -1 | -1 |
| G: -4243.27934 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10508.73545 HOMO: -6.93618 LUMO: 2.00004 factor:1 | 1 (-1.09041) | 1 | 1 |
| G: -4243.27934 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10508.71823 HOMO: -6.50896 LUMO: 1.73609 factor:1 | 1 (-1.07319) | -1 | -1 |
| G: -4243.27934 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10508.97554 HOMO: -6.69672 LUMO: 2.37283 factor:1 | 1 (-1.33050) | 1 | 1 |
| G: -4243.27934 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10508.90569 HOMO: -6.65591 LUMO: 2.20684 factor:1 | 1 (-1.26065) | 1 | 1 |
| G: -4243.27934 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10507.95329 HOMO: -6.23957 LUMO: 1.78507 factor:1 | 1 (-0.30825) | -1 | -1 |
| G: -4243.27934 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10508.08306 HOMO: -6.35114 LUMO: 1.92112 factor:1 | 1 (-0.43802) | -1 | -1 |
| G: -4243.27934 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10508.13767 HOMO: -6.53617 LUMO: 1.75241 factor:1 | 1 (-0.49263) | -1 | -1 |
| G: -4243.27934 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10508.05394 HOMO: -6.60420 LUMO: 1.78779 factor:1 | 1 (-0.40891) | 1 | 1 |
| G: -4243.27934 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10508.88142 HOMO: -7.40422 LUMO: -0.97145 factor:1 | 1 (-1.23638) | -1 | -1 |
| G: -4243.27934 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10508.72740 HOMO: -6.80013 LUMO: -0.69117 factor:1 | 1 (-1.08236) | -1 | -1 |
| G: -4243.27934 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10508.82658 HOMO: -6.68040 LUMO: -0.47076 factor:1 | 1 (-1.18155) | -1 | -1 |
| G: -4243.27934 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10509.12980 HOMO: -7.20285 LUMO: -0.66124 factor:1 | 1 (-1.48476) | -1 | -1 |
| G: -4243.27934 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10509.30311 HOMO: -6.82734 LUMO: -0.60137 factor:1 | 1 (-1.65807) | -1 | -1 |
| G: -4243.27934 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10509.95578 HOMO: -7.18653 LUMO: 0.59321 factor:1 | 1 (-2.31074) | -1 | -1 |
| G: -4243.27934 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10509.69716 HOMO: -7.29265 LUMO: 0.48164 factor:1 | 1 (-2.05212) | -1 | -1 |
| G: -4243.27934 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10509.02468 HOMO: -6.63414 LUMO: -0.25034 factor:1 | 1 (-1.37964) | -1 | -1 |
| G: -4243.27934 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10509.93341 HOMO: -7.20285 LUMO: 0.53879 factor:1 | 1 (-2.28837) | -1 | -1 |
| G: -4243.27934 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10509.13410 HOMO: -6.46815 LUMO: -0.21769 factor:1 | 1 (-1.48906) | -1 | -1 |
| G: -4243.27934 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10508.91872 HOMO: -6.57971 LUMO: -0.18776 factor:1 | 1 (-1.27368) | -1 | -1 |
| G: -4243.27934 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10507.90763 HOMO: -6.90897 LUMO: 1.91296 factor:1 | 1 (-0.26259) | 1 | 1 |
| G: -4243.27934 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10508.18165 HOMO: -6.67495 LUMO: 2.04358 factor:1 | 1 (-0.53661) | 1 | 1 |
| G: -4243.27934 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10508.04594 HOMO: -6.94162 LUMO: 1.73881 factor:1 | 1 (-0.40091) | 1 | 1 |
| G: -4243.27934 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10508.05985 HOMO: -6.73482 LUMO: 1.95922 factor:1 | 1 (-0.41481) | 1 | 1 |
| G: -4243.27934 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10507.77516 HOMO: -6.70489 LUMO: 2.04358 factor:1 | 1 (-0.13012) | 1 | 1 |
| G: -4243.27934 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10507.95740 HOMO: -7.04231 LUMO: 1.79323 factor:1 | 1 (-0.31236) | 1 | 1 |
| G: -4243.27934 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10507.96143 HOMO: -6.68584 LUMO: 1.60275 factor:1 | 1 (-0.31639) | 1 | 1 |
| G: -4243.27934 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10507.96872 HOMO: -6.40556 LUMO: 1.45581 factor:1 | 1 (-0.32368) | -1 | -1 |
| G: -4243.27934 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10508.10856 HOMO: -6.94979 LUMO: 2.16603 factor:1 | 1 (-0.46352) | 1 | 1 |
| G: -4243.27934 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10507.90796 HOMO: -6.84911 LUMO: 1.89935 factor:1 | 1 (-0.26292) | 1 | 1 |
| G: -4243.27934 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10508.06448 HOMO: -6.22052 LUMO: 1.57282 factor:1 | 1 (-0.41944) | -1 | -1 |
| G: -4243.27934 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10507.75372 HOMO: -6.51168 LUMO: 2.10072 factor:1 | 1 (-0.10868) | -1 | -1 |
| G: -4243.27934 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10508.11830 HOMO: -7.03686 LUMO: 2.12249 factor:1 | 1 (-0.47326) | 1 | 1 |
| G: -4243.27934 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10508.00660 HOMO: -6.84094 LUMO: 1.63268 factor:1 | 1 (-0.36156) | 1 | 1 |
| G: -4243.27934 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10507.88249 HOMO: -6.75387 LUMO: 1.72248 factor:1 | 1 (-0.23745) | 1 | 1 |
| G: -4243.27934 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10507.94075 HOMO: -6.86271 LUMO: 1.68711 factor:1 | 1 (-0.29571) | 1 | 1 |
| G: -4243.27934 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10507.93680 HOMO: -6.84094 LUMO: 2.02997 factor:1 | 1 (-0.29176) | 1 | 1 |
| G: -4243.27934 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10508.08214 HOMO: -6.80557 LUMO: 2.02725 factor:1 | 1 (-0.43710) | 1 | 1 |
| G: -4243.27934 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10507.81721 HOMO: -6.38651 LUMO: 1.53472 factor:1 | 1 (-0.17217) | -1 | -1 |
| G: -4243.27934 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10509.28327 HOMO: -7.51306 LUMO: 0.28572 factor:1 | 1 (-1.63823) | -1 | -1 |
| G: -4243.27934 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10508.55306 HOMO: -6.97972 LUMO: -0.74287 factor:1 | 1 (-0.90802) | -1 | -1 |
| G: -4243.27934 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10508.64974 HOMO: -6.83822 LUMO: -0.65852 factor:1 | 1 (-1.00470) | -1 | -1 |
| G: -4243.27934 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10508.81630 HOMO: -6.71305 LUMO: -0.49525 factor:1 | 1 (-1.17126) | -1 | -1 |
| G: -4243.27934 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10509.04030 HOMO: -6.60692 LUMO: -0.22313 factor:1 | 1 (-1.39526) | -1 | -1 |
| G: -4243.27934 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10509.81392 HOMO: -7.20013 LUMO: 0.55239 factor:1 | 1 (-2.16888) | -1 | -1 |
| G: -4243.27934 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10508.84476 HOMO: -6.60420 LUMO: -0.28028 factor:1 | 1 (-1.19972) | -1 | -1 |
| G: -4243.27934 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10508.98052 HOMO: -6.69128 LUMO: -0.30477 factor:1 | 1 (-1.33548) | -1 | -1 |
| G: -4243.27934 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10508.83252 HOMO: -6.65591 LUMO: -0.25579 factor:1 | 1 (-1.18748) | -1 | -1 |
| G: -4243.27934 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10507.85683 HOMO: -6.69128 LUMO: 1.70888 factor:1 | 1 (-0.21179) | 1 | 1 |
| G: -4243.27934 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10507.91947 HOMO: -6.50080 LUMO: 1.87759 factor:1 | 1 (-0.27443) | -1 | -1 |
| G: -4243.27934 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10507.94028 HOMO: -6.85727 LUMO: 1.99187 factor:1 | 1 (-0.29524) | 1 | 1 |
| G: -4243.27934 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10508.02181 HOMO: -6.58788 LUMO: 1.79051 factor:1 | 1 (-0.37677) | 1 | 1 |
| G: -4243.27934 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10507.87952 HOMO: -6.64230 LUMO: 2.16058 factor:1 | 1 (-0.23448) | 1 | 1 |
| G: -4243.27934 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10507.79911 HOMO: -6.58788 LUMO: 2.10616 factor:1 | 1 (-0.15407) | 1 | 1 |
| G: -4243.27934 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10508.62125 HOMO: -7.01782 LUMO: 2.13609 factor:1 | 1 (-0.97621) | 1 | 1 |
| G: -4243.27934 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10508.45344 HOMO: -6.31304 LUMO: 2.31841 factor:1 | 1 (-0.80840) | -1 | -1 |
| G: -4243.27934 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10508.54843 HOMO: -6.94979 LUMO: 2.07895 factor:1 | 1 (-0.90339) | 1 | 1 |
| G: -4243.27934 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10508.72073 HOMO: -6.88992 LUMO: 2.28031 factor:1 | 1 (-1.07569) | 1 | 1 |
| G: -4243.27934 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10508.73385 HOMO: -6.66407 LUMO: 2.07623 factor:1 | 1 (-1.08881) | 1 | 1 |
| G: -4243.27934 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10508.69091 HOMO: -6.52529 LUMO: 1.70071 factor:1 | 1 (-1.04587) | -1 | -1 |
| G: -4243.27934 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10507.84874 HOMO: -6.58788 LUMO: 1.57282 factor:1 | 1 (-0.20370) | -1 | -1 |
| G: -4243.27934 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10507.81391 HOMO: -6.55250 LUMO: 1.95378 factor:1 | 1 (-0.16887) | -1 | -1 |
| G: -4243.27934 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10507.89688 HOMO: -6.24773 LUMO: 1.77962 factor:1 | 1 (-0.25184) | -1 | -1 |
| G: -4243.27934 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10507.65062 HOMO: -6.31304 LUMO: 2.18507 factor:1 | 1 (-0.00558) | -1 | -1 |
| G: -4243.27934 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10507.60809 HOMO: -6.18243 LUMO: 2.01636 factor:1 | -1 (0.03695) | -1 | -1 |
| G: -4243.27934 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10508.00690 HOMO: -6.99877 LUMO: 2.14970 factor:1 | 1 (-0.36186) | 1 | 1 |
| G: -4243.27934 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10507.82409 HOMO: -6.72665 LUMO: 2.07079 factor:1 | 1 (-0.17905) | 1 | 1 |
| G: -4243.27934 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10507.77968 HOMO: -6.36202 LUMO: 2.17419 factor:1 | 1 (-0.13464) | -1 | -1 |
| G: -4243.27934 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10507.59807 HOMO: -6.78652 LUMO: 2.05718 factor:1 | -1 (0.04697) | 1 | -1 |
| G: -4243.27934 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10507.73854 HOMO: -6.87360 LUMO: 2.34290 factor:1 | 1 (-0.09350) | 1 | 1 |
| G: -4243.27934 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10508.46195 HOMO: -6.62053 LUMO: 1.89391 factor:1 | 1 (-0.81691) | 1 | 1 |
| G: -4243.27934 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10508.63845 HOMO: -6.58788 LUMO: 1.83133 factor:1 | 1 (-0.99341) | 1 | 1 |
| G: -4243.27934 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10508.77769 HOMO: -7.08584 LUMO: 1.91568 factor:1 | 1 (-1.13265) | 1 | 1 |
| G: -4243.27934 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10508.51556 HOMO: -6.56883 LUMO: 1.81228 factor:1 | 1 (-0.87052) | 1 | 1 |
| G: -4243.27934 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10508.67020 HOMO: -6.66135 LUMO: 1.92384 factor:1 | 1 (-1.02516) | 1 | 1 |
| G: -4243.27934 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10508.71352 HOMO: -6.64502 LUMO: 2.15786 factor:1 | 1 (-1.06848) | 1 | 1 |
| G: -4243.27934 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10508.03963 HOMO: -6.71305 LUMO: 1.91840 factor:1 | 1 (-0.39459) | 1 | 1 |
| G: -4243.27934 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10508.17215 HOMO: -6.44094 LUMO: 1.74425 factor:1 | 1 (-0.52711) | -1 | -1 |
| G: -4243.27934 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10508.19762 HOMO: -6.51985 LUMO: 1.84221 factor:1 | 1 (-0.55258) | -1 | -1 |
| G: -4243.27934 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10509.04175 HOMO: -6.63414 LUMO: -0.24762 factor:1 | 1 (-1.39671) | -1 | -1 |
| G: -4243.27934 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10508.65945 HOMO: -6.60420 LUMO: -0.22585 factor:1 | 1 (-1.01441) | -1 | -1 |
| G: -4243.27934 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10509.82992 HOMO: -7.19741 LUMO: 0.58232 factor:1 | 1 (-2.18488) | -1 | -1 |
| G: -4243.27934 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10508.61442 HOMO: -6.77019 LUMO: -0.56872 factor:1 | 1 (-0.96938) | -1 | -1 |
| G: -4243.27934 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10509.44651 HOMO: -7.46136 LUMO: 0.28844 factor:1 | 1 (-1.80148) | -1 | -1 |
| G: -4243.27934 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10508.78628 HOMO: -6.60420 LUMO: -0.54151 factor:1 | 1 (-1.14125) | -1 | -1 |
| G: -4243.27934 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10508.68386 HOMO: -6.53890 LUMO: -0.46531 factor:1 | 1 (-1.03882) | -1 | -1 |
| G: -4243.27934 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10508.47409 HOMO: -6.81645 LUMO: -0.57144 factor:1 | 1 (-0.82905) | -1 | -1 |
| G: -4243.27934 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10509.41187 HOMO: -7.48041 LUMO: 0.28572 factor:1 | 1 (-1.76684) | -1 | -1 |
| G: -4243.27934 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10508.78348 HOMO: -6.75659 LUMO: -0.45715 factor:1 | 1 (-1.13844) | -1 | -1 |
| G: -4243.27934 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10508.77208 HOMO: -6.66135 LUMO: -0.41906 factor:1 | 1 (-1.12704) | -1 | -1 |
| G: -4243.27934 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10509.00909 HOMO: -6.55794 LUMO: -0.27483 factor:1 | 1 (-1.36405) | -1 | -1 |
| G: -4243.27934 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10509.22700 HOMO: -7.07496 LUMO: -0.63403 factor:1 | 1 (-1.58196) | -1 | -1 |
| G: -4243.27934 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10509.82723 HOMO: -7.12394 LUMO: 0.53334 factor:1 | 1 (-2.18219) | -1 | -1 |
| G: -4243.27934 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10508.64329 HOMO: -6.53617 LUMO: -0.25579 factor:1 | 1 (-0.99825) | -1 | -1 |
| G: -4243.27934 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10508.94087 HOMO: -6.50896 LUMO: -0.25034 factor:1 | 1 (-1.29583) | -1 | -1 |
| G: -4243.27934 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10509.22548 HOMO: -7.17564 LUMO: -0.68573 factor:1 | 1 (-1.58044) | -1 | -1 |
| G: -4243.27934 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10508.97440 HOMO: -6.53617 LUMO: -0.30749 factor:1 | 1 (-1.32936) | -1 | -1 |
| G: -4243.27934 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10508.80528 HOMO: -6.55522 LUMO: -0.30749 factor:1 | 1 (-1.16024) | -1 | -1 |
| G: -4243.27934 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10509.19236 HOMO: -7.05591 LUMO: -0.71022 factor:1 | 1 (-1.54732) | -1 | -1 |
| G: -4243.27934 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10509.22621 HOMO: -7.17564 LUMO: -0.69933 factor:1 | 1 (-1.58117) | -1 | -1 |
| G: -4243.27934 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10509.22033 HOMO: -6.78380 LUMO: -0.67756 factor:1 | 1 (-1.57529) | -1 | -1 |
| G: -4243.27934 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10507.85620 HOMO: -6.62325 LUMO: 2.02725 factor:1 | 1 (-0.21116) | 1 | 1 |
| G: -4243.27934 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10507.61598 HOMO: -6.63414 LUMO: 1.91296 factor:1 | -1 (0.02906) | 1 | -1 |
| G: -4243.27934 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10507.83225 HOMO: -6.83278 LUMO: 1.65717 factor:1 | 1 (-0.18721) | 1 | 1 |
| G: -4243.27934 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10507.66621 HOMO: -6.66407 LUMO: 1.95650 factor:1 | 1 (-0.02117) | 1 | 1 |
| G: -4243.27934 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10507.68066 HOMO: -6.61237 LUMO: 2.11432 factor:1 | 1 (-0.03562) | 1 | 1 |
| G: -4243.27934 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10507.47810 HOMO: -6.62053 LUMO: 2.09256 factor:1 | -1 (0.16694) | 1 | -1 |
| G: -4243.27934 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10507.78801 HOMO: -6.78652 LUMO: 2.13609 factor:1 | 1 (-0.14297) | 1 | 1 |
| G: -4243.27934 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10507.85340 HOMO: -6.94707 LUMO: 1.81772 factor:1 | 1 (-0.20836) | 1 | 1 |
| G: -4243.27934 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10507.72558 HOMO: -6.85183 LUMO: 2.12793 factor:1 | 1 (-0.08055) | 1 | 1 |
| G: -4243.27934 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10507.84170 HOMO: -6.81101 LUMO: 1.83949 factor:1 | 1 (-0.19666) | 1 | 1 |
| G: -4243.27934 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10507.97373 HOMO: -6.98788 LUMO: 2.16058 factor:1 | 1 (-0.32869) | 1 | 1 |
| G: -4243.27934 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10507.86910 HOMO: -6.62869 LUMO: 2.00820 factor:1 | 1 (-0.22406) | 1 | 1 |
| G: -4243.27934 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10507.77399 HOMO: -6.34025 LUMO: 2.25855 factor:1 | 1 (-0.12895) | -1 | -1 |
| G: -4243.27934 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10507.60134 HOMO: -6.01372 LUMO: 2.01636 factor:1 | -1 (0.04370) | -1 | -1 |
| G: -4243.27934 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10507.73813 HOMO: -6.89264 LUMO: 2.27487 factor:1 | 1 (-0.09309) | 1 | 1 |
| G: -4243.27934 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10507.65478 HOMO: -6.53073 LUMO: 2.20684 factor:1 | 1 (-0.00974) | -1 | -1 |
| G: -4243.27934 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10507.84072 HOMO: -6.83278 LUMO: 1.53744 factor:1 | 1 (-0.19568) | -1 | -1 |
| G: -4243.27934 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10507.91873 HOMO: -6.41917 LUMO: 1.82316 factor:1 | 1 (-0.27369) | -1 | -1 |
| G: -4243.27934 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10507.77688 HOMO: -6.56339 LUMO: 1.63813 factor:1 | 1 (-0.13184) | -1 | -1 |
| G: -4243.27934 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10508.10312 HOMO: -6.88992 LUMO: 1.65173 factor:1 | 1 (-0.45808) | 1 | 1 |
| G: -4243.27934 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10507.89783 HOMO: -6.63141 LUMO: 1.92112 factor:1 | 1 (-0.25279) | 1 | 1 |
| G: -4243.27934 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10507.96611 HOMO: -6.83822 LUMO: 1.88847 factor:1 | 1 (-0.32107) | 1 | 1 |
| G: -4243.27934 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10508.07348 HOMO: -6.84638 LUMO: 1.90480 factor:1 | 1 (-0.42844) | 1 | 1 |
| G: -4243.27934 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10508.02355 HOMO: -6.82462 LUMO: 1.70888 factor:1 | 1 (-0.37851) | 1 | 1 |
| G: -4243.27934 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10508.19234 HOMO: -6.82734 LUMO: 2.12521 factor:1 | 1 (-0.54730) | 1 | 1 |
| G: -4243.27934 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10508.00948 HOMO: -6.94435 LUMO: 1.87214 factor:1 | 1 (-0.36444) | 1 | 1 |
| G: -4243.27934 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10508.81023 HOMO: -6.98516 LUMO: 2.51433 factor:1 | 1 (-1.16519) | 1 | 1 |
| G: -4243.27934 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10508.72511 HOMO: -6.74026 LUMO: 2.15514 factor:1 | 1 (-1.08007) | 1 | 1 |
| G: -4243.27934 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10508.89870 HOMO: -6.93618 LUMO: 2.54426 factor:1 | 1 (-1.25366) | 1 | 1 |
| G: -4243.27934 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10508.59477 HOMO: -6.28583 LUMO: 2.53610 factor:1 | 1 (-0.94973) | -1 | -1 |
| G: -4243.27934 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10508.58810 HOMO: -6.56883 LUMO: 1.94834 factor:1 | 1 (-0.94307) | 1 | 1 |
| G: -4243.27934 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10508.81184 HOMO: -7.08584 LUMO: 1.99187 factor:1 | 1 (-1.16680) | 1 | 1 |
| G: -4243.27934 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10507.67116 HOMO: -6.19059 LUMO: 1.99732 factor:1 | 1 (-0.02612) | -1 | -1 |
| G: -4243.27934 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10507.85470 HOMO: -6.78108 LUMO: 2.03813 factor:1 | 1 (-0.20966) | 1 | 1 |
| G: -4243.27934 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10507.97490 HOMO: -6.82189 LUMO: 1.77418 factor:1 | 1 (-0.32986) | 1 | 1 |
| G: -4243.27934 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10508.72367 HOMO: -6.45454 LUMO: 1.78779 factor:1 | 1 (-1.07863) | -1 | -1 |
| G: -4243.27934 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10508.75943 HOMO: -6.84366 LUMO: 1.77690 factor:1 | 1 (-1.11439) | 1 | 1 |
| G: -4243.27934 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10508.76343 HOMO: -6.74026 LUMO: 1.67622 factor:1 | 1 (-1.11839) | 1 | 1 |
| G: -4243.27934 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10508.91393 HOMO: -6.76475 LUMO: 2.40277 factor:1 | 1 (-1.26889) | 1 | 1 |
| G: -4243.27934 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10507.64757 HOMO: -6.65863 LUMO: 1.86670 factor:1 | 1 (-0.00253) | 1 | 1 |
| G: -4243.27934 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10507.88733 HOMO: -6.50080 LUMO: 1.93201 factor:1 | 1 (-0.24229) | -1 | -1 |
| G: -4243.27934 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10507.74686 HOMO: -6.34842 LUMO: 1.70888 factor:1 | 1 (-0.10183) | -1 | -1 |
| G: -4243.27934 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10507.94777 HOMO: -6.60692 LUMO: 2.20140 factor:1 | 1 (-0.30273) | 1 | 1 |
| G: -4243.27934 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10507.81065 HOMO: -6.74026 LUMO: 2.14970 factor:1 | 1 (-0.16561) | 1 | 1 |
| G: -4243.27934 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10507.71105 HOMO: -6.63686 LUMO: 2.17419 factor:1 | 1 (-0.06601) | 1 | 1 |
| G: -4243.27934 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10507.64256 HOMO: -6.81917 LUMO: 2.10072 factor:1 | -1 (0.00248) | 1 | -1 |
| G: -4243.27934 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10507.82804 HOMO: -6.92802 LUMO: 2.04358 factor:1 | 1 (-0.18300) | 1 | 1 |
| G: -4243.27934 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10508.64430 HOMO: -6.56067 LUMO: -0.47620 factor:1 | 1 (-0.99926) | -1 | -1 |
| G: -4243.27934 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10508.50780 HOMO: -6.56611 LUMO: -0.77008 factor:1 | 1 (-0.86276) | -1 | -1 |
| G: -4243.27934 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10508.80909 HOMO: -6.78380 LUMO: -0.64763 factor:1 | 1 (-1.16405) | -1 | -1 |
| G: -4243.27934 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10509.02746 HOMO: -6.51985 LUMO: -0.24490 factor:1 | 1 (-1.38242) | -1 | -1 |
| G: -4243.27934 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10508.85045 HOMO: -6.52529 LUMO: -0.27483 factor:1 | 1 (-1.20541) | -1 | -1 |
| G: -4243.27934 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10509.07195 HOMO: -7.10489 LUMO: -0.62586 factor:1 | 1 (-1.42691) | -1 | -1 |
| G: -4243.27934 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10509.64099 HOMO: -7.18108 LUMO: 0.48980 factor:1 | 1 (-1.99596) | -1 | -1 |
| G: -4243.27934 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10509.23435 HOMO: -7.14299 LUMO: -0.63947 factor:1 | 1 (-1.58931) | -1 | -1 |
| G: -4243.27934 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10508.63102 HOMO: -6.70761 LUMO: -0.54423 factor:1 | 1 (-0.98598) | -1 | -1 |
| G: -4243.27934 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10508.80539 HOMO: -7.32258 LUMO: -1.03675 factor:1 | 1 (-1.16035) | -1 | -1 |
| G: -4243.27934 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10508.79458 HOMO: -6.65046 LUMO: -0.41361 factor:1 | 1 (-1.14955) | -1 | -1 |
| G: -4243.27934 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10508.52429 HOMO: -6.76475 LUMO: -0.60137 factor:1 | 1 (-0.87925) | -1 | -1 |
| G: -4243.27934 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10508.64683 HOMO: -6.77836 LUMO: -0.54423 factor:1 | 1 (-1.00179) | -1 | -1 |
| G: -4243.27934 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10509.29157 HOMO: -7.52395 LUMO: 0.26395 factor:1 | 1 (-1.64653) | -1 | -1 |
| G: -4243.27934 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10508.61074 HOMO: -6.93890 LUMO: -0.72382 factor:1 | 1 (-0.96570) | -1 | -1 |
| G: -4243.27934 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10508.82503 HOMO: -6.72938 LUMO: -0.47348 factor:1 | 1 (-1.17999) | -1 | -1 |
| G: -4243.27934 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10508.56536 HOMO: -6.66951 LUMO: -0.40817 factor:1 | 1 (-0.92032) | -1 | -1 |
| G: -4243.27934 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10509.04460 HOMO: -6.60420 LUMO: -0.19320 factor:1 | 1 (-1.39956) | -1 | -1 |
| G: -4243.27934 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10508.85508 HOMO: -6.67495 LUMO: -0.27211 factor:1 | 1 (-1.21004) | -1 | -1 |
| G: -4243.27934 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10509.13244 HOMO: -7.23823 LUMO: -0.62858 factor:1 | 1 (-1.48740) | -1 | -1 |
| G: -4243.27934 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10509.68091 HOMO: -7.27088 LUMO: 0.53334 factor:1 | 1 (-2.03587) | -1 | -1 |
| G: -4243.27934 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10509.82960 HOMO: -7.20013 LUMO: 0.59049 factor:1 | 1 (-2.18456) | -1 | -1 |
| G: -4243.27934 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10508.82082 HOMO: -6.60148 LUMO: -0.20953 factor:1 | 1 (-1.17578) | -1 | -1 |
| G: -4243.27934 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10508.63747 HOMO: -6.69400 LUMO: -0.51974 factor:1 | 1 (-0.99243) | -1 | -1 |
| G: -4243.27934 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10508.88697 HOMO: -7.40422 LUMO: -0.98777 factor:1 | 1 (-1.24193) | -1 | -1 |
| G: -4243.27934 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10508.63306 HOMO: -6.88176 LUMO: -0.71022 factor:1 | 1 (-0.98802) | -1 | -1 |
| G: -4243.27934 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10508.64664 HOMO: -6.86271 LUMO: -0.59321 factor:1 | 1 (-1.00160) | -1 | -1 |
| G: -4243.27934 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10508.43297 HOMO: -6.73754 LUMO: -0.55239 factor:1 | 1 (-0.78793) | -1 | -1 |
| G: -4243.27934 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10507.89372 HOMO: -6.71033 LUMO: 1.57010 factor:1 | 1 (-0.24868) | -1 | -1 |
| G: -4243.27934 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10508.03484 HOMO: -6.69672 LUMO: 1.68711 factor:1 | 1 (-0.38980) | 1 | 1 |
| G: -4243.27934 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10508.00333 HOMO: -6.67495 LUMO: 2.03813 factor:1 | 1 (-0.35829) | 1 | 1 |
| G: -4243.27934 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10507.84044 HOMO: -6.54434 LUMO: 1.83677 factor:1 | 1 (-0.19540) | -1 | -1 |
| G: -4243.27934 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10507.99158 HOMO: -6.57155 LUMO: 1.77146 factor:1 | 1 (-0.34654) | 1 | 1 |
| G: -4243.27934 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10508.07275 HOMO: -6.76747 LUMO: 1.87759 factor:1 | 1 (-0.42771) | 1 | 1 |
| G: -4243.27934 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10507.98622 HOMO: -6.58243 LUMO: 1.61364 factor:1 | 1 (-0.34118) | 1 | 1 |
| G: -4243.27934 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10507.85043 HOMO: -6.61781 LUMO: 2.13881 factor:1 | 1 (-0.20539) | 1 | 1 |
| G: -4243.27934 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10507.71848 HOMO: -6.62597 LUMO: 2.00276 factor:1 | 1 (-0.07344) | 1 | 1 |
| G: -4243.27934 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10507.66866 HOMO: -7.01237 LUMO: 1.95922 factor:1 | 1 (-0.02362) | 1 | 1 |
| G: -4243.27934 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10507.97207 HOMO: -7.03959 LUMO: 2.16875 factor:1 | 1 (-0.32703) | 1 | 1 |
| G: -4243.27934 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10507.77652 HOMO: -6.83278 LUMO: 1.91296 factor:1 | 1 (-0.13149) | 1 | 1 |
| G: -4243.27934 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10507.62338 HOMO: -6.40012 LUMO: 1.95650 factor:1 | -1 (0.02166) | -1 | -1 |
| G: -4243.27934 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10507.89977 HOMO: -6.50080 LUMO: 1.73337 factor:1 | 1 (-0.25473) | -1 | -1 |
| G: -4243.27934 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10508.04671 HOMO: -6.95795 LUMO: 2.28848 factor:1 | 1 (-0.40167) | 1 | 1 |
| G: -4243.27934 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10507.54338 HOMO: -6.63686 LUMO: 2.20140 factor:1 | -1 (0.10166) | 1 | -1 |
| G: -4243.27934 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10507.54115 HOMO: -6.57427 LUMO: 1.87214 factor:1 | -1 (0.10389) | 1 | -1 |
| G: -4243.27934 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10507.34237 HOMO: -6.38379 LUMO: 2.32113 factor:1 | -1 (0.30267) | -1 | -1 |
| G: -4243.27934 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10508.65583 HOMO: -6.63958 LUMO: 2.04902 factor:1 | 1 (-1.01079) | 1 | 1 |
| G: -4243.27934 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10508.38737 HOMO: -6.70216 LUMO: 1.93201 factor:1 | 1 (-0.74233) | 1 | 1 |
| G: -4243.27934 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10508.59910 HOMO: -6.80557 LUMO: 2.23678 factor:1 | 1 (-0.95406) | 1 | 1 |
| G: -4243.27934 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10508.76457 HOMO: -6.72938 LUMO: 2.28304 factor:1 | 1 (-1.11953) | 1 | 1 |
| G: -4243.27934 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10508.52908 HOMO: -6.56067 LUMO: 1.66806 factor:1 | 1 (-0.88404) | -1 | -1 |
| G: -4243.27934 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10508.67766 HOMO: -6.95523 LUMO: 2.33474 factor:1 | 1 (-1.03262) | 1 | 1 |
| G: -4243.27934 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10508.17525 HOMO: -6.59876 LUMO: 2.30480 factor:1 | 1 (-0.53021) | 1 | 1 |
| G: -4243.27934 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10508.69877 HOMO: -6.87360 LUMO: 1.75786 factor:1 | 1 (-1.05373) | 1 | 1 |
| G: -4243.27934 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10507.81527 HOMO: -7.06408 LUMO: 1.99187 factor:1 | 1 (-0.17023) | 1 | 1 |
| G: -4243.27934 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10507.71592 HOMO: -6.95795 LUMO: 1.88847 factor:1 | 1 (-0.07089) | 1 | 1 |
| G: -4243.27934 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10507.84978 HOMO: -6.85455 LUMO: 1.63813 factor:1 | 1 (-0.20474) | 1 | 1 |
| G: -4243.27934 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10508.01147 HOMO: -7.09129 LUMO: 2.31569 factor:1 | 1 (-0.36643) | 1 | 1 |
| G: -4243.27934 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10507.97767 HOMO: -6.91441 LUMO: 1.68983 factor:1 | 1 (-0.33263) | 1 | 1 |
| G: -4243.27934 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10507.67190 HOMO: -6.89809 LUMO: 2.23678 factor:1 | 1 (-0.02686) | 1 | 1 |
| G: -4243.27934 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10507.63682 HOMO: -6.78652 LUMO: 1.98371 factor:1 | -1 (0.00822) | 1 | -1 |
| G: -4243.27934 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10507.69500 HOMO: -6.94707 LUMO: 2.23678 factor:1 | 1 (-0.04996) | 1 | 1 |
| G: -4243.27934 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10507.80814 HOMO: -7.07224 LUMO: 2.13337 factor:1 | 1 (-0.16311) | 1 | 1 |
| G: -4243.27934 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10507.73987 HOMO: -6.94979 LUMO: 2.28031 factor:1 | 1 (-0.09483) | 1 | 1 |
| G: -4243.27934 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10507.77119 HOMO: -6.60965 LUMO: 2.20412 factor:1 | 1 (-0.12615) | 1 | 1 |
| G: -4243.27934 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10507.61081 HOMO: -6.87360 LUMO: 2.40277 factor:1 | -1 (0.03423) | 1 | -1 |
| G: -4243.27934 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10507.55777 HOMO: -6.92802 LUMO: 1.89663 factor:1 | -1 (0.08727) | 1 | -1 |
| G: -4243.27934 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10507.77149 HOMO: -6.88448 LUMO: 2.02725 factor:1 | 1 (-0.12645) | 1 | 1 |
| G: -4243.27934 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10507.93013 HOMO: -6.69128 LUMO: 1.55105 factor:1 | 1 (-0.28509) | -1 | -1 |
| G: -4243.27934 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10507.81574 HOMO: -6.54978 LUMO: 1.93201 factor:1 | 1 (-0.17070) | -1 | -1 |
| G: -4243.27934 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10507.79857 HOMO: -6.19331 LUMO: 1.46941 factor:1 | 1 (-0.15353) | -1 | -1 |
| G: -4243.27934 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10507.90842 HOMO: -6.55794 LUMO: 1.89663 factor:1 | 1 (-0.26338) | -1 | -1 |
| G: -4243.27934 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10507.60795 HOMO: -6.07630 LUMO: 1.94289 factor:1 | -1 (0.03709) | -1 | -1 |
| G: -4243.27934 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10509.44260 HOMO: -7.46408 LUMO: 0.31565 factor:1 | 1 (-1.79756) | -1 | -1 |
| G: -4243.27934 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10508.47681 HOMO: -6.63958 LUMO: -0.61770 factor:1 | 1 (-0.83177) | -1 | -1 |
| G: -4243.27934 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10508.60459 HOMO: -6.81101 LUMO: -0.57960 factor:1 | 1 (-0.95956) | -1 | -1 |
| G: -4243.27934 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10508.65796 HOMO: -6.74298 LUMO: -0.57960 factor:1 | 1 (-1.01292) | -1 | -1 |
| G: -4243.27934 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10508.45520 HOMO: -6.63686 LUMO: -0.42994 factor:1 | 1 (-0.81016) | -1 | -1 |
| G: -4243.27934 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10508.65023 HOMO: -6.60965 LUMO: -0.41089 factor:1 | 1 (-1.00519) | -1 | -1 |
| G: -4243.27934 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10508.49567 HOMO: -6.60692 LUMO: -0.80274 factor:1 | 1 (-0.85063) | -1 | -1 |
| G: -4243.27934 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10508.64484 HOMO: -6.58788 LUMO: -0.78097 factor:1 | 1 (-0.99980) | -1 | -1 |
| G: -4243.27934 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10508.61496 HOMO: -6.67767 LUMO: -0.48436 factor:1 | 1 (-0.96992) | -1 | -1 |
| G: -4243.27934 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10508.77858 HOMO: -6.63141 LUMO: -0.40545 factor:1 | 1 (-1.13354) | -1 | -1 |
| G: -4243.27934 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10508.48212 HOMO: -6.62053 LUMO: -0.83811 factor:1 | 1 (-0.83708) | -1 | -1 |
| G: -4243.27934 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10508.98727 HOMO: -6.59604 LUMO: -0.35375 factor:1 | 1 (-1.34223) | -1 | -1 |
| G: -4243.27934 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10508.76574 HOMO: -6.34297 LUMO: -0.39729 factor:1 | 1 (-1.12070) | -1 | -1 |
| G: -4243.27934 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10507.92646 HOMO: -6.67223 LUMO: 1.97827 factor:1 | 1 (-0.28142) | 1 | 1 |
| G: -4243.27934 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10507.60183 HOMO: -6.40012 LUMO: 1.89935 factor:1 | -1 (0.04321) | -1 | -1 |
| G: -4243.27934 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10507.47192 HOMO: -6.74842 LUMO: 1.97283 factor:1 | -1 (0.17312) | 1 | -1 |
| G: -4243.27934 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10507.67206 HOMO: -6.76747 LUMO: 2.17147 factor:1 | 1 (-0.02702) | 1 | 1 |
| G: -4243.27934 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10507.81228 HOMO: -6.72121 LUMO: 1.55649 factor:1 | 1 (-0.16724) | -1 | -1 |
| G: -4243.27934 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10507.74986 HOMO: -6.97700 LUMO: 2.04085 factor:1 | 1 (-0.10482) | 1 | 1 |
| G: -4243.27934 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10507.57970 HOMO: -7.06680 LUMO: 2.04085 factor:1 | -1 (0.06533) | 1 | -1 |
| G: -4243.27934 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10507.88624 HOMO: -7.09673 LUMO: 2.35106 factor:1 | 1 (-0.24120) | 1 | 1 |
| G: -4243.27934 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10507.68782 HOMO: -6.83006 LUMO: 2.14970 factor:1 | 1 (-0.04278) | 1 | 1 |
| G: -4243.27934 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10507.48479 HOMO: -6.72665 LUMO: 2.20140 factor:1 | -1 (0.16025) | 1 | -1 |
| G: -4243.27934 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10507.25671 HOMO: -6.77291 LUMO: 2.34562 factor:1 | -1 (0.38833) | 1 | -1 |
| G: -4243.27934 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10507.57892 HOMO: -6.73754 LUMO: 2.00276 factor:1 | -1 (0.06612) | 1 | -1 |
| G: -4243.27934 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10507.63848 HOMO: -7.04231 LUMO: 1.92112 factor:1 | -1 (0.00656) | 1 | -1 |
| G: -4243.27934 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10507.82801 HOMO: -6.83822 LUMO: 1.72248 factor:1 | 1 (-0.18297) | 1 | 1 |
| G: -4243.27934 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10507.57911 HOMO: -6.57971 LUMO: 2.16603 factor:1 | -1 (0.06593) | 1 | -1 |
| G: -4243.27934 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10507.72088 HOMO: -6.80013 LUMO: 1.88575 factor:1 | 1 (-0.07584) | 1 | 1 |
| G: -4243.27934 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10508.00935 HOMO: -6.93618 LUMO: 2.18235 factor:1 | 1 (-0.36431) | 1 | 1 |
| G: -4243.27934 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10507.54724 HOMO: -6.54706 LUMO: 1.91024 factor:1 | -1 (0.09780) | -1 | -1 |
| G: -4243.27934 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10507.83002 HOMO: -7.06952 LUMO: 2.18507 factor:1 | 1 (-0.18498) | 1 | 1 |
| G: -4243.27934 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10507.83176 HOMO: -7.05047 LUMO: 1.82044 factor:1 | 1 (-0.18672) | 1 | 1 |
| G: -4243.27934 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10507.87228 HOMO: -6.87632 LUMO: 1.92657 factor:1 | 1 (-0.22724) | 1 | 1 |
| G: -4243.27934 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10507.60681 HOMO: -6.58788 LUMO: 1.91568 factor:1 | -1 (0.03823) | 1 | -1 |
| G: -4243.27934 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10507.65554 HOMO: -7.17292 LUMO: 1.90752 factor:1 | 1 (-0.01050) | 1 | 1 |
| G: -4243.27934 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10507.88812 HOMO: -6.93890 LUMO: 1.80684 factor:1 | 1 (-0.24308) | 1 | 1 |
| G: -4243.27934 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10507.95900 HOMO: -7.10761 LUMO: 2.20956 factor:1 | 1 (-0.31396) | 1 | 1 |
| G: -4243.27934 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10507.48308 HOMO: -6.85727 LUMO: 2.13609 factor:1 | -1 (0.16196) | 1 | -1 |
| G: -4243.27934 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10508.04722 HOMO: -6.64502 LUMO: 1.38506 factor:1 | 1 (-0.40218) | -1 | -1 |
| G: -4243.27934 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10507.95272 HOMO: -6.87360 LUMO: 1.15648 factor:1 | 1 (-0.30768) | -1 | -1 |
| G: -4243.27934 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10508.74041 HOMO: -6.67223 LUMO: 2.07351 factor:1 | 1 (-1.09537) | 1 | 1 |
| G: -4243.27934 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10508.49134 HOMO: -6.29671 LUMO: 2.43270 factor:1 | 1 (-0.84630) | -1 | -1 |
| G: -4243.27934 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10508.75197 HOMO: -6.90897 LUMO: 2.28848 factor:1 | 1 (-1.10693) | 1 | 1 |
| G: -4243.27934 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10508.79151 HOMO: -7.04231 LUMO: 1.70071 factor:1 | 1 (-1.14647) | 1 | 1 |
| G: -4243.27934 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10508.00589 HOMO: -6.69944 LUMO: 1.94834 factor:1 | 1 (-0.36085) | 1 | 1 |
| G: -4243.27934 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10507.44280 HOMO: -6.56067 LUMO: 2.20956 factor:1 | -1 (0.20224) | -1 | -1 |
| G: -4243.27934 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10507.61492 HOMO: -6.65046 LUMO: 2.06807 factor:1 | -1 (0.03012) | 1 | -1 |
| G: -4243.27934 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10507.72001 HOMO: -7.08584 LUMO: 1.98915 factor:1 | 1 (-0.07497) | 1 | 1 |
| G: -4243.27934 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10508.53052 HOMO: -6.69400 LUMO: 2.09256 factor:1 | 1 (-0.88549) | 1 | 1 |
| G: -4243.27934 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10508.69983 HOMO: -6.62869 LUMO: 2.16331 factor:1 | 1 (-1.05479) | 1 | 1 |
| G: -4243.27934 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10508.54576 HOMO: -6.85183 LUMO: 2.16058 factor:1 | 1 (-0.90072) | 1 | 1 |
| G: -4243.27934 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10508.58321 HOMO: -6.54706 LUMO: 1.92384 factor:1 | 1 (-0.93817) | -1 | -1 |
| G: -4243.27934 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10508.81429 HOMO: -6.84366 LUMO: 2.48984 factor:1 | 1 (-1.16925) | 1 | 1 |
| G: -4243.27934 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10508.81146 HOMO: -6.77291 LUMO: 2.46263 factor:1 | 1 (-1.16642) | 1 | 1 |
| G: -4243.27934 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10508.60917 HOMO: -7.01782 LUMO: 2.31025 factor:1 | 1 (-0.96413) | 1 | 1 |
| G: -4243.27934 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10508.69159 HOMO: -6.94707 LUMO: 2.29664 factor:1 | 1 (-1.04655) | 1 | 1 |
| G: -4243.27934 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10508.36064 HOMO: -6.64230 LUMO: 1.97283 factor:1 | 1 (-0.71561) | 1 | 1 |
| G: -4243.27934 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10508.32331 HOMO: -6.47359 LUMO: 2.20412 factor:1 | 1 (-0.67827) | -1 | -1 |
| G: -4243.27934 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10508.53833 HOMO: -6.90625 LUMO: 1.92384 factor:1 | 1 (-0.89330) | 1 | 1 |
| G: -4243.27934 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10507.64847 HOMO: -7.17020 LUMO: 2.06807 factor:1 | 1 (-0.00343) | 1 | 1 |
| G: -4243.27934 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10507.62814 HOMO: -6.65046 LUMO: 2.20956 factor:1 | -1 (0.01690) | 1 | -1 |
| G: -4243.27934 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10507.81288 HOMO: -7.07496 LUMO: 1.82861 factor:1 | 1 (-0.16784) | 1 | 1 |
| G: -4243.27934 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10507.54177 HOMO: -6.83006 LUMO: 2.14970 factor:1 | -1 (0.10327) | 1 | -1 |
| G: -4243.27934 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10507.83171 HOMO: -6.92802 LUMO: 1.99187 factor:1 | 1 (-0.18667) | 1 | 1 |
| G: -4243.27934 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10507.60085 HOMO: -6.69672 LUMO: 2.36739 factor:1 | -1 (0.04419) | 1 | -1 |
| G: -4243.27934 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10507.83130 HOMO: -7.13755 LUMO: 2.00276 factor:1 | 1 (-0.18626) | 1 | 1 |
| G: -4243.27934 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10507.69165 HOMO: -6.92530 LUMO: 2.25582 factor:1 | 1 (-0.04661) | 1 | 1 |
| G: -4243.27934 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10507.79092 HOMO: -6.77564 LUMO: 1.97827 factor:1 | 1 (-0.14588) | 1 | 1 |
| G: -4243.27934 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10507.79073 HOMO: -6.87904 LUMO: 1.60003 factor:1 | 1 (-0.14569) | 1 | 1 |
| G: -4243.27934 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10507.94200 HOMO: -6.62869 LUMO: 1.90480 factor:1 | 1 (-0.29696) | 1 | 1 |
| G: -4243.27934 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10508.04839 HOMO: -6.71033 LUMO: 1.54833 factor:1 | 1 (-0.40335) | -1 | -1 |
| G: -4243.27934 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10508.08429 HOMO: -6.74298 LUMO: 1.47486 factor:1 | 1 (-0.43925) | -1 | -1 |
| G: -4243.27934 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10507.80964 HOMO: -6.77019 LUMO: 1.90480 factor:1 | 1 (-0.16460) | 1 | 1 |
| G: -4243.27934 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10507.74526 HOMO: -6.70489 LUMO: 1.99459 factor:1 | 1 (-0.10022) | 1 | 1 |
| G: -4243.27934 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10508.62851 HOMO: -6.73482 LUMO: 2.08711 factor:1 | 1 (-0.98347) | 1 | 1 |
| G: -4243.27934 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10508.58285 HOMO: -6.46543 LUMO: 1.73881 factor:1 | 1 (-0.93781) | -1 | -1 |
| G: -4243.27934 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10508.60402 HOMO: -6.96067 LUMO: 2.26127 factor:1 | 1 (-0.95898) | 1 | 1 |
| G: -4243.27934 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10508.72688 HOMO: -6.67767 LUMO: 2.10616 factor:1 | 1 (-1.08184) | 1 | 1 |
| G: -4243.27934 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10508.43450 HOMO: -6.28855 LUMO: 2.35923 factor:1 | 1 (-0.78946) | -1 | -1 |
| G: -4243.27934 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10508.88844 HOMO: -6.80285 LUMO: 1.62724 factor:1 | 1 (-1.24340) | 1 | 1 |
| G: -4243.27934 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10508.45373 HOMO: -6.85455 LUMO: 2.23133 factor:1 | 1 (-0.80870) | 1 | 1 |
| G: -4243.27934 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10508.23942 HOMO: -6.51713 LUMO: 2.33474 factor:1 | 1 (-0.59438) | -1 | -1 |
| G: -4243.27934 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10508.32530 HOMO: -6.88176 LUMO: 2.15242 factor:1 | 1 (-0.68026) | 1 | 1 |
| G: -4243.27934 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10508.18951 HOMO: -6.54434 LUMO: 2.32113 factor:1 | 1 (-0.54447) | -1 | -1 |
| G: -4243.27934 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10508.08682 HOMO: -6.62597 LUMO: 2.24222 factor:1 | 1 (-0.44178) | 1 | 1 |
| G: -4243.27934 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10508.54359 HOMO: -6.74570 LUMO: 2.19868 factor:1 | 1 (-0.89855) | 1 | 1 |
| G: -4243.27934 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10508.26943 HOMO: -6.62869 LUMO: 1.98915 factor:1 | 1 (-0.62439) | 1 | 1 |
| G: -4243.27934 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10508.33833 HOMO: -6.64502 LUMO: 2.13881 factor:1 | 1 (-0.69329) | 1 | 1 |
| G: -4243.27934 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10508.54756 HOMO: -6.95795 LUMO: 1.82316 factor:1 | 1 (-0.90252) | 1 | 1 |
| G: -4243.27934 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10508.68860 HOMO: -6.77291 LUMO: 1.36329 factor:1 | 1 (-1.04356) | -1 | -1 |
| G: -4243.27934 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10508.61349 HOMO: -6.45726 LUMO: 1.73064 factor:1 | 1 (-0.96845) | -1 | -1 |
| G: -4243.27934 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10508.54862 HOMO: -6.49264 LUMO: 1.77418 factor:1 | 1 (-0.90358) | -1 | -1 |
| G: -4243.27934 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10507.75554 HOMO: -6.60420 LUMO: 2.20956 factor:1 | 1 (-0.11051) | 1 | 1 |
| G: -4243.27934 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10507.73100 HOMO: -6.56067 LUMO: 2.05718 factor:1 | 1 (-0.08596) | -1 | -1 |
| G: -4243.27934 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10507.85582 HOMO: -6.62597 LUMO: 1.70343 factor:1 | 1 (-0.21078) | 1 | 1 |
| G: -4243.27934 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10507.87802 HOMO: -6.69400 LUMO: 2.16875 factor:1 | 1 (-0.23298) | 1 | 1 |
| G: -4243.27934 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10507.77481 HOMO: -6.63958 LUMO: 2.11977 factor:1 | 1 (-0.12977) | 1 | 1 |
| G: -4243.27934 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10507.58098 HOMO: -6.92802 LUMO: 1.82044 factor:1 | -1 (0.06406) | 1 | -1 |
| G: -4243.27934 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10507.53960 HOMO: -6.56339 LUMO: 2.30480 factor:1 | -1 (0.10544) | -1 | -1 |
| G: -4243.27934 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10507.52504 HOMO: -6.63958 LUMO: 1.91024 factor:1 | -1 (0.12000) | 1 | -1 |
| G: -4243.27934 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10507.78553 HOMO: -6.93074 LUMO: 2.05446 factor:1 | 1 (-0.14049) | 1 | 1 |
| G: -4243.27934 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10507.75285 HOMO: -6.61509 LUMO: 2.03813 factor:1 | 1 (-0.10781) | 1 | 1 |
| G: -4243.27934 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10507.58618 HOMO: -6.61237 LUMO: 1.91296 factor:1 | -1 (0.05886) | 1 | -1 |
| G: -4243.27934 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10507.96420 HOMO: -6.86815 LUMO: 1.95378 factor:1 | 1 (-0.31916) | 1 | 1 |
| G: -4243.27934 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10507.73593 HOMO: -6.63686 LUMO: 1.70888 factor:1 | 1 (-0.09089) | 1 | 1 |
| G: -4243.27934 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10507.60245 HOMO: -6.57971 LUMO: 2.20140 factor:1 | -1 (0.04259) | 1 | -1 |
| G: -4243.27934 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10507.45306 HOMO: -6.41100 LUMO: 1.96738 factor:1 | -1 (0.19198) | -1 | -1 |
| G: -4243.27934 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10507.86115 HOMO: -6.90081 LUMO: 1.65989 factor:1 | 1 (-0.21611) | 1 | 1 |
| G: -4243.27934 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10507.56302 HOMO: -6.68312 LUMO: 1.97827 factor:1 | -1 (0.08202) | 1 | -1 |
| G: -4243.27934 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10507.63198 HOMO: -6.65318 LUMO: 2.10888 factor:1 | -1 (0.01306) | 1 | -1 |
| G: -4243.27934 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10507.52991 HOMO: -6.62053 LUMO: 2.28848 factor:1 | -1 (0.11513) | 1 | -1 |
| G: -4243.27934 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10507.53015 HOMO: -6.65863 LUMO: 2.29664 factor:1 | -1 (0.11489) | 1 | -1 |
| G: -4243.27934 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10507.37701 HOMO: -6.63958 LUMO: 2.07623 factor:1 | -1 (0.26803) | 1 | -1 |
| G: -4243.27934 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10507.72648 HOMO: -6.58243 LUMO: 2.20684 factor:1 | 1 (-0.08144) | 1 | 1 |
| G: -4243.27934 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10507.58471 HOMO: -6.59332 LUMO: 2.05174 factor:1 | -1 (0.06033) | 1 | -1 |
| G: -4243.27934 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10507.73843 HOMO: -6.95251 LUMO: 2.20140 factor:1 | 1 (-0.09339) | 1 | 1 |
| G: -4243.27934 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10508.51156 HOMO: -6.84638 LUMO: 2.39732 factor:1 | 1 (-0.86652) | 1 | 1 |
| G: -4243.27934 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10508.62699 HOMO: -6.86815 LUMO: 2.47896 factor:1 | 1 (-0.98195) | 1 | 1 |
| G: -4243.27934 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10508.71194 HOMO: -7.00693 LUMO: 2.43270 factor:1 | 1 (-1.06690) | 1 | 1 |
| G: -4243.27934 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10508.31621 HOMO: -6.58788 LUMO: 2.30208 factor:1 | 1 (-0.67117) | 1 | 1 |
| G: -4243.27934 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10508.23283 HOMO: -6.63958 LUMO: 2.28031 factor:1 | 1 (-0.58779) | 1 | 1 |
| G: -4243.27934 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10508.14241 HOMO: -6.74570 LUMO: 2.28304 factor:1 | 1 (-0.49737) | 1 | 1 |
| G: -4243.27934 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10508.46584 HOMO: -6.78380 LUMO: 2.16331 factor:1 | 1 (-0.82080) | 1 | 1 |
| G: -4243.27934 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10508.33253 HOMO: -6.52529 LUMO: 2.05718 factor:1 | 1 (-0.68750) | -1 | -1 |
| G: -4243.27934 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10507.84782 HOMO: -6.41644 LUMO: 1.65445 factor:1 | 1 (-0.20278) | -1 | -1 |
| G: -4243.27934 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10507.77217 HOMO: -6.34570 LUMO: 1.22451 factor:1 | 1 (-0.12713) | -1 | -1 |
| G: -4243.27934 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10507.63620 HOMO: -6.14433 LUMO: 1.85582 factor:1 | -1 (0.00884) | -1 | -1 |
| G: -4243.27934 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10507.46087 HOMO: -6.62053 LUMO: 1.92112 factor:1 | -1 (0.18417) | 1 | -1 |
| G: -4243.27934 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10507.87827 HOMO: -6.63414 LUMO: 1.61908 factor:1 | 1 (-0.23323) | 1 | 1 |
| G: -4243.27934 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10507.88725 HOMO: -6.75931 LUMO: 1.87214 factor:1 | 1 (-0.24221) | 1 | 1 |
| G: -4243.27934 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10507.89723 HOMO: -6.55794 LUMO: 1.77418 factor:1 | 1 (-0.25220) | -1 | -1 |
| G: -4243.27934 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10507.90240 HOMO: -6.52801 LUMO: 1.82044 factor:1 | 1 (-0.25737) | -1 | -1 |
| G: -4243.27934 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10507.72651 HOMO: -6.77564 LUMO: 1.97827 factor:1 | 1 (-0.08147) | 1 | 1 |
| G: -4243.27934 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10507.82480 HOMO: -6.93890 LUMO: 1.81228 factor:1 | 1 (-0.17976) | 1 | 1 |
| G: -4243.27934 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10507.85519 HOMO: -6.85455 LUMO: 1.75513 factor:1 | 1 (-0.21015) | 1 | 1 |
| G: -4243.27934 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10507.89391 HOMO: -6.86815 LUMO: 1.64629 factor:1 | 1 (-0.24888) | 1 | 1 |
| G: -4243.27934 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10507.93691 HOMO: -6.98516 LUMO: 1.84765 factor:1 | 1 (-0.29187) | 1 | 1 |
| G: -4243.27934 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10507.57492 HOMO: -6.04637 LUMO: 1.94017 factor:1 | -1 (0.07012) | -1 | -1 |
| G: -4243.27934 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10507.52599 HOMO: -6.86271 LUMO: 2.11977 factor:1 | -1 (0.11905) | 1 | -1 |
| G: -4243.27934 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10507.61954 HOMO: -6.72938 LUMO: 2.11160 factor:1 | -1 (0.02550) | 1 | -1 |
| G: -4243.27934 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10507.80727 HOMO: -7.01782 LUMO: 2.13609 factor:1 | 1 (-0.16223) | 1 | 1 |
| G: -4243.27934 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10507.57470 HOMO: -6.18515 LUMO: 2.04630 factor:1 | -1 (0.07034) | -1 | -1 |
| G: -4243.27934 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10507.60422 HOMO: -6.60965 LUMO: 2.17147 factor:1 | -1 (0.04082) | 1 | -1 |
| G: -4243.27934 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10507.69715 HOMO: -6.87360 LUMO: 2.35378 factor:1 | 1 (-0.05211) | 1 | 1 |
| G: -4243.27934 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10507.47124 HOMO: -6.72938 LUMO: 2.20140 factor:1 | -1 (0.17380) | 1 | -1 |
| G: -4243.27934 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10507.62014 HOMO: -6.88448 LUMO: 2.54154 factor:1 | -1 (0.02490) | 1 | -1 |
| G: -4243.27934 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10507.66645 HOMO: -6.87087 LUMO: 2.16058 factor:1 | 1 (-0.02142) | 1 | 1 |
| G: -4243.27934 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10507.85797 HOMO: -7.11306 LUMO: 2.04085 factor:1 | 1 (-0.21293) | 1 | 1 |
| G: -4243.27934 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10507.93204 HOMO: -6.66951 LUMO: 1.68438 factor:1 | 1 (-0.28700) | 1 | 1 |
| G: -4243.27934 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10507.98970 HOMO: -7.08312 LUMO: 2.19324 factor:1 | 1 (-0.34466) | 1 | 1 |
| G: -4243.27934 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10507.58765 HOMO: -6.69128 LUMO: 2.13881 factor:1 | -1 (0.05739) | 1 | -1 |
| G: -4243.27934 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10508.47325 HOMO: -6.80285 LUMO: 2.16603 factor:1 | 1 (-0.82821) | 1 | 1 |
| G: -4243.27934 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10508.65412 HOMO: -6.82189 LUMO: 2.46807 factor:1 | 1 (-1.00908) | 1 | 1 |
| G: -4243.27934 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10508.69317 HOMO: -6.78652 LUMO: 2.12521 factor:1 | 1 (-1.04813) | 1 | 1 |
| G: -4243.27934 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10508.44680 HOMO: -6.47903 LUMO: 1.70071 factor:1 | 1 (-0.80176) | -1 | -1 |
| G: -4243.27934 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10507.80458 HOMO: -6.37019 LUMO: 1.24356 factor:1 | 1 (-0.15954) | -1 | -1 |
| G: -4243.27934 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10507.90972 HOMO: -6.69400 LUMO: 1.67350 factor:1 | 1 (-0.26469) | 1 | 1 |
| G: -4243.27934 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10509.30317 HOMO: -7.51851 LUMO: 0.27756 factor:1 | 1 (-1.65813) | -1 | -1 |
| G: -4243.27934 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10508.51365 HOMO: -6.95795 LUMO: -0.72110 factor:1 | 1 (-0.86861) | -1 | -1 |
| G: -4243.27934 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10508.56209 HOMO: -6.88720 LUMO: -0.67484 factor:1 | 1 (-0.91705) | -1 | -1 |
| G: -4243.27934 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10508.59529 HOMO: -6.83550 LUMO: -0.57144 factor:1 | 1 (-0.95025) | -1 | -1 |
| G: -4243.27934 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10508.44677 HOMO: -6.80285 LUMO: -0.57144 factor:1 | 1 (-0.80173) | -1 | -1 |
| G: -4243.27934 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10508.64465 HOMO: -6.76475 LUMO: -0.53062 factor:1 | 1 (-0.99961) | -1 | -1 |
| G: -4243.27934 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10507.77500 HOMO: -6.66951 LUMO: 1.74969 factor:1 | 1 (-0.12996) | 1 | 1 |
| G: -4243.27934 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10507.73573 HOMO: -6.53345 LUMO: 1.89935 factor:1 | 1 (-0.09070) | -1 | -1 |
| G: -4243.27934 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10507.61998 HOMO: -6.65046 LUMO: 2.01364 factor:1 | -1 (0.02506) | 1 | -1 |
| G: -4243.27934 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10507.55472 HOMO: -6.64230 LUMO: 2.11977 factor:1 | -1 (0.09031) | 1 | -1 |
| G: -4243.27934 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10507.29423 HOMO: -6.44910 LUMO: 2.13337 factor:1 | -1 (0.35081) | -1 | -1 |
| G: -4243.27934 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10507.59783 HOMO: -7.05591 LUMO: 1.98915 factor:1 | -1 (0.04721) | 1 | -1 |
| G: -4243.27934 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10508.63624 HOMO: -7.02326 LUMO: 2.49256 factor:1 | 1 (-0.99120) | 1 | 1 |
| G: -4243.27934 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10508.41216 HOMO: -6.32937 LUMO: 2.51161 factor:1 | 1 (-0.76712) | -1 | -1 |
| G: -4243.27934 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10508.47178 HOMO: -6.96067 LUMO: 2.20140 factor:1 | 1 (-0.82674) | 1 | 1 |
| G: -4243.27934 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10508.72032 HOMO: -6.97972 LUMO: 2.55243 factor:1 | 1 (-1.07529) | 1 | 1 |
| G: -4243.27934 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10508.57831 HOMO: -6.72665 LUMO: 2.46535 factor:1 | 1 (-0.93327) | 1 | 1 |
| G: -4243.27934 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10508.27207 HOMO: -6.41917 LUMO: 2.35106 factor:1 | 1 (-0.62703) | -1 | -1 |
| G: -4243.27934 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10508.29672 HOMO: -6.75114 LUMO: 2.32929 factor:1 | 1 (-0.65169) | 1 | 1 |
| G: -4243.27934 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10508.63368 HOMO: -6.91713 LUMO: 2.27215 factor:1 | 1 (-0.98864) | 1 | 1 |
| G: -4243.27934 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10508.44130 HOMO: -6.54978 LUMO: 2.00276 factor:1 | 1 (-0.79626) | -1 | -1 |
| G: -4243.27934 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10508.45341 HOMO: -6.62325 LUMO: 2.05990 factor:1 | 1 (-0.80837) | 1 | 1 |
| G: -4243.27934 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10507.69971 HOMO: -6.86271 LUMO: 2.14970 factor:1 | 1 (-0.05467) | 1 | 1 |
| G: -4243.27934 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10507.44403 HOMO: -6.77564 LUMO: 2.25855 factor:1 | -1 (0.20101) | 1 | -1 |
| G: -4243.27934 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10507.47935 HOMO: -6.71305 LUMO: 1.94561 factor:1 | -1 (0.16569) | 1 | -1 |
| G: -4243.27934 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10507.59595 HOMO: -6.75659 LUMO: 1.94561 factor:1 | -1 (0.04909) | 1 | -1 |
| G: -4243.27934 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10507.52765 HOMO: -6.94979 LUMO: 2.33474 factor:1 | -1 (0.11739) | 1 | -1 |
| G: -4243.27934 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10507.59206 HOMO: -6.85727 LUMO: 2.50345 factor:1 | -1 (0.05298) | 1 | -1 |
| G: -4243.27934 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10507.45151 HOMO: -6.87360 LUMO: 2.43270 factor:1 | -1 (0.19353) | 1 | -1 |
| G: -4243.27934 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10507.25679 HOMO: -6.57427 LUMO: 2.46807 factor:1 | -1 (0.38825) | 1 | -1 |
| G: -4243.27934 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10507.65731 HOMO: -7.16204 LUMO: 2.15242 factor:1 | 1 (-0.01227) | 1 | 1 |
| G: -4243.27934 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10507.47557 HOMO: -6.62869 LUMO: 2.11432 factor:1 | -1 (0.16947) | 1 | -1 |
| G: -4243.27934 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10507.58610 HOMO: -7.05591 LUMO: 2.26671 factor:1 | -1 (0.05894) | 1 | -1 |
| G: -4243.27934 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10507.60732 HOMO: -7.13483 LUMO: 1.47758 factor:1 | -1 (0.03771) | -1 | -1 |
| G: -4243.27934 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10507.75682 HOMO: -6.72938 LUMO: 1.57282 factor:1 | 1 (-0.11178) | -1 | -1 |
| G: -4243.27934 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10507.47519 HOMO: -6.17426 LUMO: 1.81228 factor:1 | -1 (0.16985) | -1 | -1 |
| G: -4243.27934 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10507.47908 HOMO: -6.65318 LUMO: 1.93473 factor:1 | -1 (0.16596) | 1 | -1 |
| G: -4243.27934 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10507.17578 HOMO: -6.18515 LUMO: 2.01364 factor:1 | -1 (0.46926) | -1 | -1 |
| G: -4243.27934 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10507.81204 HOMO: -7.05591 LUMO: 2.13337 factor:1 | 1 (-0.16700) | 1 | 1 |
| G: -4243.27934 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10507.55818 HOMO: -6.90897 LUMO: 2.29664 factor:1 | -1 (0.08686) | 1 | -1 |
| G: -4243.27934 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10507.82420 HOMO: -7.11034 LUMO: 2.17147 factor:1 | 1 (-0.17916) | 1 | 1 |
| G: -4243.27934 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10507.65954 HOMO: -6.82734 LUMO: 2.26671 factor:1 | 1 (-0.01450) | 1 | 1 |
| G: -4243.27934 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10507.23496 HOMO: -6.34842 LUMO: 2.34562 factor:1 | -1 (0.41008) | -1 | -1 |
| G: -4243.27934 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10507.42411 HOMO: -6.62053 LUMO: 2.22861 factor:1 | -1 (0.22093) | 1 | -1 |
| G: -4243.27934 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10507.35717 HOMO: -6.80557 LUMO: 2.07079 factor:1 | -1 (0.28787) | 1 | -1 |
| G: -4243.27934 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10507.21834 HOMO: -6.60692 LUMO: 2.46263 factor:1 | -1 (0.42670) | 1 | -1 |
| G: -4243.27934 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10507.57649 HOMO: -7.02054 LUMO: 2.08711 factor:1 | -1 (0.06855) | 1 | -1 |
| G: -4243.27934 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10508.48530 HOMO: -6.78652 LUMO: 2.02453 factor:1 | 1 (-0.84026) | 1 | 1 |
| G: -4243.27934 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10508.29566 HOMO: -6.51168 LUMO: 2.06534 factor:1 | 1 (-0.65062) | -1 | -1 |
| G: -4243.27934 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10508.40783 HOMO: -6.50080 LUMO: 2.01636 factor:1 | 1 (-0.76279) | -1 | -1 |
| G: -4243.27934 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10508.43286 HOMO: -6.54434 LUMO: 1.84493 factor:1 | 1 (-0.78782) | -1 | -1 |
| G: -4243.27934 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10508.55385 HOMO: -6.47087 LUMO: 1.76330 factor:1 | 1 (-0.90881) | -1 | -1 |
| G: -4243.27934 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10508.61610 HOMO: -6.78924 LUMO: 2.39460 factor:1 | 1 (-0.97107) | 1 | 1 |
| G: -4243.27934 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10508.26380 HOMO: -6.59876 LUMO: 1.84493 factor:1 | 1 (-0.61876) | 1 | 1 |
| G: -4243.27934 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10508.30872 HOMO: -6.41644 LUMO: 2.05174 factor:1 | 1 (-0.66369) | -1 | -1 |
| G: -4243.27934 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10508.20472 HOMO: -6.52257 LUMO: 2.11160 factor:1 | 1 (-0.55968) | -1 | -1 |
| G: -4243.27934 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10508.61009 HOMO: -6.90897 LUMO: 2.34018 factor:1 | 1 (-0.96505) | 1 | 1 |
| G: -4243.27934 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10508.53550 HOMO: -6.97428 LUMO: 1.86126 factor:1 | 1 (-0.89047) | 1 | 1 |
| G: -4243.27934 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10507.62654 HOMO: -7.13483 LUMO: 2.14698 factor:1 | -1 (0.01850) | 1 | -1 |
| G: -4243.27934 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10507.86619 HOMO: -7.16748 LUMO: 2.31841 factor:1 | 1 (-0.22115) | 1 | 1 |
| G: -4243.27934 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10507.64036 HOMO: -6.87087 LUMO: 2.38916 factor:1 | -1 (0.00468) | 1 | -1 |
| G: -4243.27934 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10507.43567 HOMO: -6.93074 LUMO: 2.42181 factor:1 | -1 (0.20936) | 1 | -1 |
| G: -4243.27934 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10507.49731 HOMO: -6.90081 LUMO: 2.00276 factor:1 | -1 (0.14773) | 1 | -1 |
| G: -4243.27934 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10507.73677 HOMO: -6.99333 LUMO: 2.03541 factor:1 | 1 (-0.09173) | 1 | 1 |
| G: -4243.27934 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10507.91288 HOMO: -6.89264 LUMO: 1.57554 factor:1 | 1 (-0.26784) | -1 | -1 |
| G: -4243.27934 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10507.90632 HOMO: -6.48175 LUMO: 1.85854 factor:1 | 1 (-0.26128) | -1 | -1 |
| G: -4243.27934 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10507.97672 HOMO: -6.69400 LUMO: 1.62452 factor:1 | 1 (-0.33168) | 1 | 1 |
| G: -4243.27934 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10507.77783 HOMO: -6.50896 LUMO: 1.88303 factor:1 | 1 (-0.13279) | -1 | -1 |
| G: -4243.27934 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10507.80986 HOMO: -6.60420 LUMO: 2.05990 factor:1 | 1 (-0.16482) | 1 | 1 |
| G: -4243.27934 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10507.84341 HOMO: -7.14299 LUMO: 2.07351 factor:1 | 1 (-0.19837) | 1 | 1 |
| G: -4243.27934 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10507.78123 HOMO: -7.06408 LUMO: 1.81228 factor:1 | 1 (-0.13619) | 1 | 1 |
| G: -4243.27934 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10507.86281 HOMO: -6.67495 LUMO: 1.79595 factor:1 | 1 (-0.21777) | 1 | 1 |
| G: -4243.27934 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10507.76319 HOMO: -6.45182 LUMO: 2.15786 factor:1 | 1 (-0.11815) | -1 | -1 |
| G: -4243.27934 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10508.26442 HOMO: -6.93346 LUMO: 2.45719 factor:1 | 1 (-0.61939) | 1 | 1 |
| G: -4243.27934 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10507.93675 HOMO: -6.50080 LUMO: 2.08167 factor:1 | 1 (-0.29171) | -1 | -1 |
| G: -4242.91430 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10509.35160 HOMO: -6.83550 LUMO: -0.67484 factor:1 | 1 (-2.07160) | -1 | -1 |
| G: -4242.91430 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10509.92018 HOMO: -7.04231 LUMO: 0.54151 factor:1 | 1 (-2.64018) | -1 | -1 |
| G: -4242.91430 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10508.27291 HOMO: -6.79740 LUMO: 1.91296 factor:1 | 1 (-0.99292) | -1 | -1 |
| G: -4242.91430 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10508.85801 HOMO: -7.35796 LUMO: -1.04220 factor:1 | 1 (-1.57802) | -1 | -1 |
| G: -4242.91430 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10508.82686 HOMO: -6.62597 LUMO: -0.44082 factor:1 | 1 (-1.54686) | -1 | -1 |
| G: -4242.91430 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10508.75926 HOMO: -6.45182 LUMO: -0.20409 factor:1 | 1 (-1.47927) | -1 | -1 |
| G: -4242.91430 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10509.24458 HOMO: -6.51168 LUMO: -0.23130 factor:1 | 1 (-1.96458) | -1 | -1 |
| G: -4242.91430 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10509.66951 HOMO: -7.14027 LUMO: 0.49797 factor:1 | 1 (-2.38951) | -1 | -1 |
| G: -4242.91430 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10509.34210 HOMO: -7.55660 LUMO: 0.24762 factor:1 | 1 (-2.06211) | -1 | -1 |
| G: -4242.91430 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10508.64726 HOMO: -6.88992 LUMO: -0.64763 factor:1 | 1 (-1.36726) | -1 | -1 |
| G: -4242.91430 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10508.88912 HOMO: -6.72665 LUMO: -0.45987 factor:1 | 1 (-1.60912) | -1 | -1 |
| G: -4242.91430 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10508.62805 HOMO: -6.72121 LUMO: -0.58232 factor:1 | 1 (-1.34805) | -1 | -1 |
| G: -4242.91430 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10509.37198 HOMO: -7.26816 LUMO: 0.32926 factor:1 | 1 (-2.09198) | -1 | -1 |
| G: -4242.91430 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10508.82977 HOMO: -6.57155 LUMO: -0.53606 factor:1 | 1 (-1.54977) | -1 | -1 |
| G: -4242.91430 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10508.52672 HOMO: -6.50896 LUMO: -0.43810 factor:1 | 1 (-1.24672) | -1 | -1 |
| G: -4242.91430 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10508.63123 HOMO: -6.73210 LUMO: -0.51430 factor:1 | 1 (-1.35124) | -1 | -1 |
| G: -4242.91430 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10508.84473 HOMO: -6.77019 LUMO: -0.62858 factor:1 | 1 (-1.56474) | -1 | -1 |
| G: -4242.91430 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10508.74745 HOMO: -6.82462 LUMO: -0.67484 factor:1 | 1 (-1.46746) | -1 | -1 |
| G: -4242.91430 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10508.52998 HOMO: -6.79740 LUMO: -0.55511 factor:1 | 1 (-1.24998) | -1 | -1 |
| G: -4242.91430 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10508.81856 HOMO: -6.79740 LUMO: -0.67756 factor:1 | 1 (-1.53856) | -1 | -1 |
| G: -4242.91430 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10508.78909 HOMO: -6.75114 LUMO: -0.55239 factor:1 | 1 (-1.50909) | -1 | -1 |
| G: -4242.91430 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10508.96248 HOMO: -6.49536 LUMO: -0.25307 factor:1 | 1 (-1.68248) | -1 | -1 |
| G: -4242.91430 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10509.17459 HOMO: -6.48992 LUMO: -0.25034 factor:1 | 1 (-1.89459) | -1 | -1 |
| G: -4242.91430 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10508.85611 HOMO: -6.52801 LUMO: -0.28028 factor:1 | 1 (-1.57611) | -1 | -1 |
| G: -4242.91430 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10509.83874 HOMO: -7.22462 LUMO: 0.52518 factor:1 | 1 (-2.55874) | -1 | -1 |
| G: -4242.91430 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10508.98289 HOMO: -6.59332 LUMO: -0.27211 factor:1 | 1 (-1.70289) | -1 | -1 |
| G: -4242.91430 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10509.21446 HOMO: -6.57427 LUMO: -0.16871 factor:1 | 1 (-1.93446) | -1 | -1 |
| G: -4242.91430 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10508.10339 HOMO: -6.71033 LUMO: 1.59187 factor:1 | 1 (-0.82339) | -1 | -1 |
| G: -4242.91430 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10508.12535 HOMO: -6.72121 LUMO: 2.00004 factor:1 | 1 (-0.84535) | -1 | -1 |
| G: -4242.91430 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10508.24679 HOMO: -6.61509 LUMO: 1.55921 factor:1 | 1 (-0.96679) | -1 | -1 |
| G: -4242.91430 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10508.24279 HOMO: -6.55250 LUMO: 1.73064 factor:1 | 1 (-0.96279) | -1 | -1 |
| G: -4242.91430 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10508.17297 HOMO: -6.66135 LUMO: 2.02181 factor:1 | 1 (-0.89297) | -1 | -1 |
| G: -4242.91430 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10507.96594 HOMO: -6.84911 LUMO: 1.98099 factor:1 | 1 (-0.68594) | -1 | -1 |
| G: -4242.91430 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10507.86738 HOMO: -6.66679 LUMO: 1.98371 factor:1 | 1 (-0.58738) | -1 | -1 |
| G: -4242.91430 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10507.98303 HOMO: -6.67495 LUMO: 2.04085 factor:1 | 1 (-0.70303) | -1 | -1 |
| G: -4242.91430 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10508.13147 HOMO: -6.89809 LUMO: 1.95106 factor:1 | 1 (-0.85147) | -1 | -1 |
| G: -4242.91430 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10508.69880 HOMO: -6.50352 LUMO: 1.88847 factor:1 | 1 (-1.41880) | -1 | -1 |
| G: -4242.91430 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10508.73545 HOMO: -6.93618 LUMO: 2.00004 factor:1 | 1 (-1.45546) | -1 | -1 |
| G: -4242.91430 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10508.71823 HOMO: -6.50896 LUMO: 1.73609 factor:1 | 1 (-1.43823) | -1 | -1 |
| G: -4242.91430 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10508.97554 HOMO: -6.69672 LUMO: 2.37283 factor:1 | 1 (-1.69554) | -1 | -1 |
| G: -4242.91430 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10508.90569 HOMO: -6.65591 LUMO: 2.20684 factor:1 | 1 (-1.62569) | -1 | -1 |
| G: -4242.91430 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10507.95329 HOMO: -6.23957 LUMO: 1.78507 factor:1 | 1 (-0.67329) | -1 | -1 |
| G: -4242.91430 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10508.08306 HOMO: -6.35114 LUMO: 1.92112 factor:1 | 1 (-0.80306) | -1 | -1 |
| G: -4242.91430 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10508.13767 HOMO: -6.53617 LUMO: 1.75241 factor:1 | 1 (-0.85768) | -1 | -1 |
| G: -4242.91430 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10508.05394 HOMO: -6.60420 LUMO: 1.78779 factor:1 | 1 (-0.77395) | -1 | -1 |
| G: -4242.91430 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10508.88142 HOMO: -7.40422 LUMO: -0.97145 factor:1 | 1 (-1.60142) | -1 | -1 |
| G: -4242.91430 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10508.72740 HOMO: -6.80013 LUMO: -0.69117 factor:1 | 1 (-1.44740) | -1 | -1 |
| G: -4242.91430 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10508.82658 HOMO: -6.68040 LUMO: -0.47076 factor:1 | 1 (-1.54659) | -1 | -1 |
| G: -4242.91430 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10509.12980 HOMO: -7.20285 LUMO: -0.66124 factor:1 | 1 (-1.84980) | -1 | -1 |
| G: -4242.91430 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10509.30311 HOMO: -6.82734 LUMO: -0.60137 factor:1 | 1 (-2.02311) | -1 | -1 |
| G: -4242.91430 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10509.95578 HOMO: -7.18653 LUMO: 0.59321 factor:1 | 1 (-2.67578) | -1 | -1 |
| G: -4242.91430 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10509.69716 HOMO: -7.29265 LUMO: 0.48164 factor:1 | 1 (-2.41716) | -1 | -1 |
| G: -4242.91430 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10509.02468 HOMO: -6.63414 LUMO: -0.25034 factor:1 | 1 (-1.74469) | -1 | -1 |
| G: -4242.91430 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10509.93341 HOMO: -7.20285 LUMO: 0.53879 factor:1 | 1 (-2.65341) | -1 | -1 |
| G: -4242.91430 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10509.13410 HOMO: -6.46815 LUMO: -0.21769 factor:1 | 1 (-1.85410) | -1 | -1 |
| G: -4242.91430 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10508.91872 HOMO: -6.57971 LUMO: -0.18776 factor:1 | 1 (-1.63872) | -1 | -1 |
| G: -4242.91430 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10507.90763 HOMO: -6.90897 LUMO: 1.91296 factor:1 | 1 (-0.62763) | -1 | -1 |
| G: -4242.91430 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10508.18165 HOMO: -6.67495 LUMO: 2.04358 factor:1 | 1 (-0.90165) | -1 | -1 |
| G: -4242.91430 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10508.04594 HOMO: -6.94162 LUMO: 1.73881 factor:1 | 1 (-0.76595) | -1 | -1 |
| G: -4242.91430 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10508.05985 HOMO: -6.73482 LUMO: 1.95922 factor:1 | 1 (-0.77985) | -1 | -1 |
| G: -4242.91430 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10507.77516 HOMO: -6.70489 LUMO: 2.04358 factor:1 | 1 (-0.49517) | -1 | -1 |
| G: -4242.91430 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10507.95740 HOMO: -7.04231 LUMO: 1.79323 factor:1 | 1 (-0.67740) | -1 | -1 |
| G: -4242.91430 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10507.96143 HOMO: -6.68584 LUMO: 1.60275 factor:1 | 1 (-0.68143) | -1 | -1 |
| G: -4242.91430 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10507.96872 HOMO: -6.40556 LUMO: 1.45581 factor:1 | 1 (-0.68872) | -1 | -1 |
| G: -4242.91430 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10508.10856 HOMO: -6.94979 LUMO: 2.16603 factor:1 | 1 (-0.82856) | -1 | -1 |
| G: -4242.91430 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10507.90796 HOMO: -6.84911 LUMO: 1.89935 factor:1 | 1 (-0.62796) | -1 | -1 |
| G: -4242.91430 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10508.06448 HOMO: -6.22052 LUMO: 1.57282 factor:1 | 1 (-0.78448) | -1 | -1 |
| G: -4242.91430 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10507.75372 HOMO: -6.51168 LUMO: 2.10072 factor:1 | 1 (-0.47372) | -1 | -1 |
| G: -4242.91430 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10508.11830 HOMO: -7.03686 LUMO: 2.12249 factor:1 | 1 (-0.83830) | -1 | -1 |
| G: -4242.91430 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10508.00660 HOMO: -6.84094 LUMO: 1.63268 factor:1 | 1 (-0.72660) | -1 | -1 |
| G: -4242.91430 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10507.88249 HOMO: -6.75387 LUMO: 1.72248 factor:1 | 1 (-0.60249) | -1 | -1 |
| G: -4242.91430 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10507.94075 HOMO: -6.86271 LUMO: 1.68711 factor:1 | 1 (-0.66075) | -1 | -1 |
| G: -4242.91430 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10507.93680 HOMO: -6.84094 LUMO: 2.02997 factor:1 | 1 (-0.65680) | -1 | -1 |
| G: -4242.91430 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10508.08214 HOMO: -6.80557 LUMO: 2.02725 factor:1 | 1 (-0.80214) | -1 | -1 |
| G: -4242.91430 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10507.81721 HOMO: -6.38651 LUMO: 1.53472 factor:1 | 1 (-0.53721) | -1 | -1 |
| G: -4242.91430 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10509.28327 HOMO: -7.51306 LUMO: 0.28572 factor:1 | 1 (-2.00328) | -1 | -1 |
| G: -4242.91430 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10508.55306 HOMO: -6.97972 LUMO: -0.74287 factor:1 | 1 (-1.27306) | -1 | -1 |
| G: -4242.91430 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10508.64974 HOMO: -6.83822 LUMO: -0.65852 factor:1 | 1 (-1.36974) | -1 | -1 |
| G: -4242.91430 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10508.81630 HOMO: -6.71305 LUMO: -0.49525 factor:1 | 1 (-1.53630) | -1 | -1 |
| G: -4242.91430 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10509.04030 HOMO: -6.60692 LUMO: -0.22313 factor:1 | 1 (-1.76030) | -1 | -1 |
| G: -4242.91430 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10509.81392 HOMO: -7.20013 LUMO: 0.55239 factor:1 | 1 (-2.53392) | -1 | -1 |
| G: -4242.91430 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10508.84476 HOMO: -6.60420 LUMO: -0.28028 factor:1 | 1 (-1.56476) | -1 | -1 |
| G: -4242.91430 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10508.98052 HOMO: -6.69128 LUMO: -0.30477 factor:1 | 1 (-1.70052) | -1 | -1 |
| G: -4242.91430 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10508.83252 HOMO: -6.65591 LUMO: -0.25579 factor:1 | 1 (-1.55252) | -1 | -1 |
| G: -4242.91430 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10507.85683 HOMO: -6.69128 LUMO: 1.70888 factor:1 | 1 (-0.57683) | -1 | -1 |
| G: -4242.91430 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10507.91947 HOMO: -6.50080 LUMO: 1.87759 factor:1 | 1 (-0.63947) | -1 | -1 |
| G: -4242.91430 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10507.94028 HOMO: -6.85727 LUMO: 1.99187 factor:1 | 1 (-0.66028) | -1 | -1 |
| G: -4242.91430 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10508.02181 HOMO: -6.58788 LUMO: 1.79051 factor:1 | 1 (-0.74181) | -1 | -1 |
| G: -4242.91430 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10507.87952 HOMO: -6.64230 LUMO: 2.16058 factor:1 | 1 (-0.59952) | -1 | -1 |
| G: -4242.91430 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10507.79911 HOMO: -6.58788 LUMO: 2.10616 factor:1 | 1 (-0.51911) | -1 | -1 |
| G: -4242.91430 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10508.62125 HOMO: -7.01782 LUMO: 2.13609 factor:1 | 1 (-1.34125) | -1 | -1 |
| G: -4242.91430 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10508.45344 HOMO: -6.31304 LUMO: 2.31841 factor:1 | 1 (-1.17344) | -1 | -1 |
| G: -4242.91430 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10508.54843 HOMO: -6.94979 LUMO: 2.07895 factor:1 | 1 (-1.26843) | -1 | -1 |
| G: -4242.91430 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10508.72073 HOMO: -6.88992 LUMO: 2.28031 factor:1 | 1 (-1.44073) | -1 | -1 |
| G: -4242.91430 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10508.73385 HOMO: -6.66407 LUMO: 2.07623 factor:1 | 1 (-1.45385) | -1 | -1 |
| G: -4242.91430 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10508.69091 HOMO: -6.52529 LUMO: 1.70071 factor:1 | 1 (-1.41091) | -1 | -1 |
| G: -4242.91430 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10507.84874 HOMO: -6.58788 LUMO: 1.57282 factor:1 | 1 (-0.56875) | -1 | -1 |
| G: -4242.91430 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10507.81391 HOMO: -6.55250 LUMO: 1.95378 factor:1 | 1 (-0.53391) | -1 | -1 |
| G: -4242.91430 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10507.89688 HOMO: -6.24773 LUMO: 1.77962 factor:1 | 1 (-0.61688) | -1 | -1 |
| G: -4242.91430 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10507.65062 HOMO: -6.31304 LUMO: 2.18507 factor:1 | 1 (-0.37062) | -1 | -1 |
| G: -4242.91430 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10507.60809 HOMO: -6.18243 LUMO: 2.01636 factor:1 | 1 (-0.32809) | -1 | -1 |
| G: -4242.91430 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10508.00690 HOMO: -6.99877 LUMO: 2.14970 factor:1 | 1 (-0.72690) | -1 | -1 |
| G: -4242.91430 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10507.82409 HOMO: -6.72665 LUMO: 2.07079 factor:1 | 1 (-0.54409) | -1 | -1 |
| G: -4242.91430 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10507.77968 HOMO: -6.36202 LUMO: 2.17419 factor:1 | 1 (-0.49968) | -1 | -1 |
| G: -4242.91430 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10507.59807 HOMO: -6.78652 LUMO: 2.05718 factor:1 | 1 (-0.31807) | -1 | -1 |
| G: -4242.91430 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10507.73854 HOMO: -6.87360 LUMO: 2.34290 factor:1 | 1 (-0.45854) | -1 | -1 |
| G: -4242.91430 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10508.46195 HOMO: -6.62053 LUMO: 1.89391 factor:1 | 1 (-1.18195) | -1 | -1 |
| G: -4242.91430 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10508.63845 HOMO: -6.58788 LUMO: 1.83133 factor:1 | 1 (-1.35845) | -1 | -1 |
| G: -4242.91430 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10508.77769 HOMO: -7.08584 LUMO: 1.91568 factor:1 | 1 (-1.49769) | 1 | 1 |
| G: -4242.91430 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10508.51556 HOMO: -6.56883 LUMO: 1.81228 factor:1 | 1 (-1.23556) | -1 | -1 |
| G: -4242.91430 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10508.67020 HOMO: -6.66135 LUMO: 1.92384 factor:1 | 1 (-1.39020) | -1 | -1 |
| G: -4242.91430 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10508.71352 HOMO: -6.64502 LUMO: 2.15786 factor:1 | 1 (-1.43352) | -1 | -1 |
| G: -4242.91430 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10508.03963 HOMO: -6.71305 LUMO: 1.91840 factor:1 | 1 (-0.75963) | -1 | -1 |
| G: -4242.91430 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10508.17215 HOMO: -6.44094 LUMO: 1.74425 factor:1 | 1 (-0.89215) | -1 | -1 |
| G: -4242.91430 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10508.19762 HOMO: -6.51985 LUMO: 1.84221 factor:1 | 1 (-0.91762) | -1 | -1 |
| G: -4242.91430 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10509.04175 HOMO: -6.63414 LUMO: -0.24762 factor:1 | 1 (-1.76175) | -1 | -1 |
| G: -4242.91430 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10508.65945 HOMO: -6.60420 LUMO: -0.22585 factor:1 | 1 (-1.37945) | -1 | -1 |
| G: -4242.91430 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10509.82992 HOMO: -7.19741 LUMO: 0.58232 factor:1 | 1 (-2.54992) | -1 | -1 |
| G: -4242.91430 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10508.61442 HOMO: -6.77019 LUMO: -0.56872 factor:1 | 1 (-1.33442) | -1 | -1 |
| G: -4242.91430 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10509.44651 HOMO: -7.46136 LUMO: 0.28844 factor:1 | 1 (-2.16652) | -1 | -1 |
| G: -4242.91430 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10508.78628 HOMO: -6.60420 LUMO: -0.54151 factor:1 | 1 (-1.50629) | -1 | -1 |
| G: -4242.91430 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10508.68386 HOMO: -6.53890 LUMO: -0.46531 factor:1 | 1 (-1.40386) | -1 | -1 |
| G: -4242.91430 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10508.47409 HOMO: -6.81645 LUMO: -0.57144 factor:1 | 1 (-1.19409) | -1 | -1 |
| G: -4242.91430 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10509.41187 HOMO: -7.48041 LUMO: 0.28572 factor:1 | 1 (-2.13188) | -1 | -1 |
| G: -4242.91430 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10508.78348 HOMO: -6.75659 LUMO: -0.45715 factor:1 | 1 (-1.50348) | -1 | -1 |
| G: -4242.91430 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10508.77208 HOMO: -6.66135 LUMO: -0.41906 factor:1 | 1 (-1.49208) | -1 | -1 |
| G: -4242.91430 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10509.00909 HOMO: -6.55794 LUMO: -0.27483 factor:1 | 1 (-1.72909) | -1 | -1 |
| G: -4242.91430 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10509.22700 HOMO: -7.07496 LUMO: -0.63403 factor:1 | 1 (-1.94700) | -1 | -1 |
| G: -4242.91430 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10509.82723 HOMO: -7.12394 LUMO: 0.53334 factor:1 | 1 (-2.54723) | -1 | -1 |
| G: -4242.91430 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10508.64329 HOMO: -6.53617 LUMO: -0.25579 factor:1 | 1 (-1.36329) | -1 | -1 |
| G: -4242.91430 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10508.94087 HOMO: -6.50896 LUMO: -0.25034 factor:1 | 1 (-1.66087) | -1 | -1 |
| G: -4242.91430 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10509.22548 HOMO: -7.17564 LUMO: -0.68573 factor:1 | 1 (-1.94548) | -1 | -1 |
| G: -4242.91430 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10508.97440 HOMO: -6.53617 LUMO: -0.30749 factor:1 | 1 (-1.69440) | -1 | -1 |
| G: -4242.91430 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10508.80528 HOMO: -6.55522 LUMO: -0.30749 factor:1 | 1 (-1.52528) | -1 | -1 |
| G: -4242.91430 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10509.19236 HOMO: -7.05591 LUMO: -0.71022 factor:1 | 1 (-1.91236) | -1 | -1 |
| G: -4242.91430 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10509.22621 HOMO: -7.17564 LUMO: -0.69933 factor:1 | 1 (-1.94621) | -1 | -1 |
| G: -4242.91430 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10509.22033 HOMO: -6.78380 LUMO: -0.67756 factor:1 | 1 (-1.94034) | -1 | -1 |
| G: -4242.91430 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10507.85620 HOMO: -6.62325 LUMO: 2.02725 factor:1 | 1 (-0.57620) | -1 | -1 |
| G: -4242.91430 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10507.61598 HOMO: -6.63414 LUMO: 1.91296 factor:1 | 1 (-0.33598) | -1 | -1 |
| G: -4242.91430 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10507.83225 HOMO: -6.83278 LUMO: 1.65717 factor:1 | 1 (-0.55226) | -1 | -1 |
| G: -4242.91430 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10507.66621 HOMO: -6.66407 LUMO: 1.95650 factor:1 | 1 (-0.38621) | -1 | -1 |
| G: -4242.91430 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10507.68066 HOMO: -6.61237 LUMO: 2.11432 factor:1 | 1 (-0.40066) | -1 | -1 |
| G: -4242.91430 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10507.47810 HOMO: -6.62053 LUMO: 2.09256 factor:1 | 1 (-0.19810) | -1 | -1 |
| G: -4242.91430 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10507.78801 HOMO: -6.78652 LUMO: 2.13609 factor:1 | 1 (-0.50801) | -1 | -1 |
| G: -4242.91430 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10507.85340 HOMO: -6.94707 LUMO: 1.81772 factor:1 | 1 (-0.57340) | -1 | -1 |
| G: -4242.91430 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10507.72558 HOMO: -6.85183 LUMO: 2.12793 factor:1 | 1 (-0.44559) | -1 | -1 |
| G: -4242.91430 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10507.84170 HOMO: -6.81101 LUMO: 1.83949 factor:1 | 1 (-0.56170) | -1 | -1 |
| G: -4242.91430 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10507.97373 HOMO: -6.98788 LUMO: 2.16058 factor:1 | 1 (-0.69373) | -1 | -1 |
| G: -4242.91430 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10507.86910 HOMO: -6.62869 LUMO: 2.00820 factor:1 | 1 (-0.58910) | -1 | -1 |
| G: -4242.91430 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10507.77399 HOMO: -6.34025 LUMO: 2.25855 factor:1 | 1 (-0.49400) | -1 | -1 |
| G: -4242.91430 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10507.60134 HOMO: -6.01372 LUMO: 2.01636 factor:1 | 1 (-0.32134) | -1 | -1 |
| G: -4242.91430 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10507.73813 HOMO: -6.89264 LUMO: 2.27487 factor:1 | 1 (-0.45813) | -1 | -1 |
| G: -4242.91430 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10507.65478 HOMO: -6.53073 LUMO: 2.20684 factor:1 | 1 (-0.37478) | -1 | -1 |
| G: -4242.91430 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10507.84072 HOMO: -6.83278 LUMO: 1.53744 factor:1 | 1 (-0.56072) | -1 | -1 |
| G: -4242.91430 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10507.91873 HOMO: -6.41917 LUMO: 1.82316 factor:1 | 1 (-0.63873) | -1 | -1 |
| G: -4242.91430 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10507.77688 HOMO: -6.56339 LUMO: 1.63813 factor:1 | 1 (-0.49688) | -1 | -1 |
| G: -4242.91430 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10508.10312 HOMO: -6.88992 LUMO: 1.65173 factor:1 | 1 (-0.82312) | -1 | -1 |
| G: -4242.91430 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10507.89783 HOMO: -6.63141 LUMO: 1.92112 factor:1 | 1 (-0.61783) | -1 | -1 |
| G: -4242.91430 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10507.96611 HOMO: -6.83822 LUMO: 1.88847 factor:1 | 1 (-0.68611) | -1 | -1 |
| G: -4242.91430 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10508.07348 HOMO: -6.84638 LUMO: 1.90480 factor:1 | 1 (-0.79348) | -1 | -1 |
| G: -4242.91430 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10508.02355 HOMO: -6.82462 LUMO: 1.70888 factor:1 | 1 (-0.74355) | -1 | -1 |
| G: -4242.91430 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10508.19234 HOMO: -6.82734 LUMO: 2.12521 factor:1 | 1 (-0.91234) | -1 | -1 |
| G: -4242.91430 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10508.00948 HOMO: -6.94435 LUMO: 1.87214 factor:1 | 1 (-0.72948) | -1 | -1 |
| G: -4242.91430 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10508.81023 HOMO: -6.98516 LUMO: 2.51433 factor:1 | 1 (-1.53023) | -1 | -1 |
| G: -4242.91430 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10508.72511 HOMO: -6.74026 LUMO: 2.15514 factor:1 | 1 (-1.44512) | -1 | -1 |
| G: -4242.91430 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10508.89870 HOMO: -6.93618 LUMO: 2.54426 factor:1 | 1 (-1.61870) | -1 | -1 |
| G: -4242.91430 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10508.59477 HOMO: -6.28583 LUMO: 2.53610 factor:1 | 1 (-1.31477) | -1 | -1 |
| G: -4242.91430 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10508.58810 HOMO: -6.56883 LUMO: 1.94834 factor:1 | 1 (-1.30811) | -1 | -1 |
| G: -4242.91430 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10508.81184 HOMO: -7.08584 LUMO: 1.99187 factor:1 | 1 (-1.53184) | 1 | 1 |
| G: -4242.91430 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10507.67116 HOMO: -6.19059 LUMO: 1.99732 factor:1 | 1 (-0.39116) | -1 | -1 |
| G: -4242.91430 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10507.85470 HOMO: -6.78108 LUMO: 2.03813 factor:1 | 1 (-0.57470) | -1 | -1 |
| G: -4242.91430 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10507.97490 HOMO: -6.82189 LUMO: 1.77418 factor:1 | 1 (-0.69490) | -1 | -1 |
| G: -4242.91430 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10508.72367 HOMO: -6.45454 LUMO: 1.78779 factor:1 | 1 (-1.44367) | -1 | -1 |
| G: -4242.91430 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10508.75943 HOMO: -6.84366 LUMO: 1.77690 factor:1 | 1 (-1.47943) | -1 | -1 |
| G: -4242.91430 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10508.76343 HOMO: -6.74026 LUMO: 1.67622 factor:1 | 1 (-1.48343) | -1 | -1 |
| G: -4242.91430 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10508.91393 HOMO: -6.76475 LUMO: 2.40277 factor:1 | 1 (-1.63393) | -1 | -1 |
| G: -4242.91430 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10507.64757 HOMO: -6.65863 LUMO: 1.86670 factor:1 | 1 (-0.36757) | -1 | -1 |
| G: -4242.91430 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10507.88733 HOMO: -6.50080 LUMO: 1.93201 factor:1 | 1 (-0.60733) | -1 | -1 |
| G: -4242.91430 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10507.74686 HOMO: -6.34842 LUMO: 1.70888 factor:1 | 1 (-0.46687) | -1 | -1 |
| G: -4242.91430 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10507.94777 HOMO: -6.60692 LUMO: 2.20140 factor:1 | 1 (-0.66777) | -1 | -1 |
| G: -4242.91430 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10507.81065 HOMO: -6.74026 LUMO: 2.14970 factor:1 | 1 (-0.53065) | -1 | -1 |
| G: -4242.91430 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10507.71105 HOMO: -6.63686 LUMO: 2.17419 factor:1 | 1 (-0.43106) | -1 | -1 |
| G: -4242.91430 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10507.64256 HOMO: -6.81917 LUMO: 2.10072 factor:1 | 1 (-0.36256) | -1 | -1 |
| G: -4242.91430 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10507.82804 HOMO: -6.92802 LUMO: 2.04358 factor:1 | 1 (-0.54804) | -1 | -1 |
| G: -4242.91430 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10508.64430 HOMO: -6.56067 LUMO: -0.47620 factor:1 | 1 (-1.36430) | -1 | -1 |
| G: -4242.91430 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10508.50780 HOMO: -6.56611 LUMO: -0.77008 factor:1 | 1 (-1.22780) | -1 | -1 |
| G: -4242.91430 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10508.80909 HOMO: -6.78380 LUMO: -0.64763 factor:1 | 1 (-1.52909) | -1 | -1 |
| G: -4242.91430 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10509.02746 HOMO: -6.51985 LUMO: -0.24490 factor:1 | 1 (-1.74746) | -1 | -1 |
| G: -4242.91430 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10508.85045 HOMO: -6.52529 LUMO: -0.27483 factor:1 | 1 (-1.57045) | -1 | -1 |
| G: -4242.91430 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10509.07195 HOMO: -7.10489 LUMO: -0.62586 factor:1 | 1 (-1.79195) | -1 | -1 |
| G: -4242.91430 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10509.64099 HOMO: -7.18108 LUMO: 0.48980 factor:1 | 1 (-2.36100) | -1 | -1 |
| G: -4242.91430 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10509.23435 HOMO: -7.14299 LUMO: -0.63947 factor:1 | 1 (-1.95435) | -1 | -1 |
| G: -4242.91430 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10508.63102 HOMO: -6.70761 LUMO: -0.54423 factor:1 | 1 (-1.35102) | -1 | -1 |
| G: -4242.91430 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10508.80539 HOMO: -7.32258 LUMO: -1.03675 factor:1 | 1 (-1.52539) | -1 | -1 |
| G: -4242.91430 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10508.79458 HOMO: -6.65046 LUMO: -0.41361 factor:1 | 1 (-1.51459) | -1 | -1 |
| G: -4242.91430 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10508.52429 HOMO: -6.76475 LUMO: -0.60137 factor:1 | 1 (-1.24430) | -1 | -1 |
| G: -4242.91430 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10508.64683 HOMO: -6.77836 LUMO: -0.54423 factor:1 | 1 (-1.36683) | -1 | -1 |
| G: -4242.91430 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10509.29157 HOMO: -7.52395 LUMO: 0.26395 factor:1 | 1 (-2.01157) | -1 | -1 |
| G: -4242.91430 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10508.61074 HOMO: -6.93890 LUMO: -0.72382 factor:1 | 1 (-1.33075) | -1 | -1 |
| G: -4242.91430 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10508.82503 HOMO: -6.72938 LUMO: -0.47348 factor:1 | 1 (-1.54504) | -1 | -1 |
| G: -4242.91430 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10508.56536 HOMO: -6.66951 LUMO: -0.40817 factor:1 | 1 (-1.28536) | -1 | -1 |
| G: -4242.91430 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10509.04460 HOMO: -6.60420 LUMO: -0.19320 factor:1 | 1 (-1.76460) | -1 | -1 |
| G: -4242.91430 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10508.85508 HOMO: -6.67495 LUMO: -0.27211 factor:1 | 1 (-1.57508) | -1 | -1 |
| G: -4242.91430 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10509.13244 HOMO: -7.23823 LUMO: -0.62858 factor:1 | 1 (-1.85244) | -1 | -1 |
| G: -4242.91430 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10509.68091 HOMO: -7.27088 LUMO: 0.53334 factor:1 | 1 (-2.40092) | -1 | -1 |
| G: -4242.91430 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10509.82960 HOMO: -7.20013 LUMO: 0.59049 factor:1 | 1 (-2.54960) | -1 | -1 |
| G: -4242.91430 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10508.82082 HOMO: -6.60148 LUMO: -0.20953 factor:1 | 1 (-1.54082) | -1 | -1 |
| G: -4242.91430 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10508.63747 HOMO: -6.69400 LUMO: -0.51974 factor:1 | 1 (-1.35747) | -1 | -1 |
| G: -4242.91430 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10508.88697 HOMO: -7.40422 LUMO: -0.98777 factor:1 | 1 (-1.60697) | -1 | -1 |
| G: -4242.91430 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10508.63306 HOMO: -6.88176 LUMO: -0.71022 factor:1 | 1 (-1.35306) | -1 | -1 |
| G: -4242.91430 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10508.64664 HOMO: -6.86271 LUMO: -0.59321 factor:1 | 1 (-1.36664) | -1 | -1 |
| G: -4242.91430 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10508.43297 HOMO: -6.73754 LUMO: -0.55239 factor:1 | 1 (-1.15297) | -1 | -1 |
| G: -4242.91430 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10507.89372 HOMO: -6.71033 LUMO: 1.57010 factor:1 | 1 (-0.61373) | -1 | -1 |
| G: -4242.91430 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10508.03484 HOMO: -6.69672 LUMO: 1.68711 factor:1 | 1 (-0.75484) | -1 | -1 |
| G: -4242.91430 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10508.00333 HOMO: -6.67495 LUMO: 2.03813 factor:1 | 1 (-0.72333) | -1 | -1 |
| G: -4242.91430 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10507.84044 HOMO: -6.54434 LUMO: 1.83677 factor:1 | 1 (-0.56045) | -1 | -1 |
| G: -4242.91430 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10507.99158 HOMO: -6.57155 LUMO: 1.77146 factor:1 | 1 (-0.71158) | -1 | -1 |
| G: -4242.91430 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10508.07275 HOMO: -6.76747 LUMO: 1.87759 factor:1 | 1 (-0.79275) | -1 | -1 |
| G: -4242.91430 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10507.98622 HOMO: -6.58243 LUMO: 1.61364 factor:1 | 1 (-0.70622) | -1 | -1 |
| G: -4242.91430 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10507.85043 HOMO: -6.61781 LUMO: 2.13881 factor:1 | 1 (-0.57043) | -1 | -1 |
| G: -4242.91430 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10507.71848 HOMO: -6.62597 LUMO: 2.00276 factor:1 | 1 (-0.43848) | -1 | -1 |
| G: -4242.91430 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10507.66866 HOMO: -7.01237 LUMO: 1.95922 factor:1 | 1 (-0.38866) | -1 | -1 |
| G: -4242.91430 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10507.97207 HOMO: -7.03959 LUMO: 2.16875 factor:1 | 1 (-0.69207) | -1 | -1 |
| G: -4242.91430 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10507.77652 HOMO: -6.83278 LUMO: 1.91296 factor:1 | 1 (-0.49653) | -1 | -1 |
| G: -4242.91430 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10507.62338 HOMO: -6.40012 LUMO: 1.95650 factor:1 | 1 (-0.34338) | -1 | -1 |
| G: -4242.91430 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10507.89977 HOMO: -6.50080 LUMO: 1.73337 factor:1 | 1 (-0.61977) | -1 | -1 |
| G: -4242.91430 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10508.04671 HOMO: -6.95795 LUMO: 2.28848 factor:1 | 1 (-0.76671) | -1 | -1 |
| G: -4242.91430 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10507.54338 HOMO: -6.63686 LUMO: 2.20140 factor:1 | 1 (-0.26338) | -1 | -1 |
| G: -4242.91430 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10507.54115 HOMO: -6.57427 LUMO: 1.87214 factor:1 | 1 (-0.26115) | -1 | -1 |
| G: -4242.91430 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10507.34237 HOMO: -6.38379 LUMO: 2.32113 factor:1 | 1 (-0.06237) | -1 | -1 |
| G: -4242.91430 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10508.65583 HOMO: -6.63958 LUMO: 2.04902 factor:1 | 1 (-1.37583) | -1 | -1 |
| G: -4242.91430 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10508.38737 HOMO: -6.70216 LUMO: 1.93201 factor:1 | 1 (-1.10737) | -1 | -1 |
| G: -4242.91430 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10508.59910 HOMO: -6.80557 LUMO: 2.23678 factor:1 | 1 (-1.31910) | -1 | -1 |
| G: -4242.91430 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10508.76457 HOMO: -6.72938 LUMO: 2.28304 factor:1 | 1 (-1.48457) | -1 | -1 |
| G: -4242.91430 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10508.52908 HOMO: -6.56067 LUMO: 1.66806 factor:1 | 1 (-1.24908) | -1 | -1 |
| G: -4242.91430 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10508.67766 HOMO: -6.95523 LUMO: 2.33474 factor:1 | 1 (-1.39766) | -1 | -1 |
| G: -4242.91430 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10508.17525 HOMO: -6.59876 LUMO: 2.30480 factor:1 | 1 (-0.89525) | -1 | -1 |
| G: -4242.91430 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10508.69877 HOMO: -6.87360 LUMO: 1.75786 factor:1 | 1 (-1.41877) | -1 | -1 |
| G: -4242.91430 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10507.81527 HOMO: -7.06408 LUMO: 1.99187 factor:1 | 1 (-0.53528) | 1 | 1 |
| G: -4242.91430 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10507.71592 HOMO: -6.95795 LUMO: 1.88847 factor:1 | 1 (-0.43593) | -1 | -1 |
| G: -4242.91430 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10507.84978 HOMO: -6.85455 LUMO: 1.63813 factor:1 | 1 (-0.56978) | -1 | -1 |
| G: -4242.91430 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10508.01147 HOMO: -7.09129 LUMO: 2.31569 factor:1 | 1 (-0.73147) | 1 | 1 |
| G: -4242.91430 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10507.97767 HOMO: -6.91441 LUMO: 1.68983 factor:1 | 1 (-0.69767) | -1 | -1 |
| G: -4242.91430 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10507.67190 HOMO: -6.89809 LUMO: 2.23678 factor:1 | 1 (-0.39190) | -1 | -1 |
| G: -4242.91430 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10507.63682 HOMO: -6.78652 LUMO: 1.98371 factor:1 | 1 (-0.35682) | -1 | -1 |
| G: -4242.91430 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10507.69500 HOMO: -6.94707 LUMO: 2.23678 factor:1 | 1 (-0.41500) | -1 | -1 |
| G: -4242.91430 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10507.80814 HOMO: -7.07224 LUMO: 2.13337 factor:1 | 1 (-0.52815) | 1 | 1 |
| G: -4242.91430 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10507.73987 HOMO: -6.94979 LUMO: 2.28031 factor:1 | 1 (-0.45987) | -1 | -1 |
| G: -4242.91430 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10507.77119 HOMO: -6.60965 LUMO: 2.20412 factor:1 | 1 (-0.49119) | -1 | -1 |
| G: -4242.91430 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10507.61081 HOMO: -6.87360 LUMO: 2.40277 factor:1 | 1 (-0.33081) | -1 | -1 |
| G: -4242.91430 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10507.55777 HOMO: -6.92802 LUMO: 1.89663 factor:1 | 1 (-0.27777) | -1 | -1 |
| G: -4242.91430 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10507.77149 HOMO: -6.88448 LUMO: 2.02725 factor:1 | 1 (-0.49149) | -1 | -1 |
| G: -4242.91430 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10507.93013 HOMO: -6.69128 LUMO: 1.55105 factor:1 | 1 (-0.65013) | -1 | -1 |
| G: -4242.91430 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10507.81574 HOMO: -6.54978 LUMO: 1.93201 factor:1 | 1 (-0.53574) | -1 | -1 |
| G: -4242.91430 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10507.79857 HOMO: -6.19331 LUMO: 1.46941 factor:1 | 1 (-0.51857) | -1 | -1 |
| G: -4242.91430 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10507.90842 HOMO: -6.55794 LUMO: 1.89663 factor:1 | 1 (-0.62842) | -1 | -1 |
| G: -4242.91430 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10507.60795 HOMO: -6.07630 LUMO: 1.94289 factor:1 | 1 (-0.32795) | -1 | -1 |
| G: -4242.91430 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10509.44260 HOMO: -7.46408 LUMO: 0.31565 factor:1 | 1 (-2.16260) | -1 | -1 |
| G: -4242.91430 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10508.47681 HOMO: -6.63958 LUMO: -0.61770 factor:1 | 1 (-1.19681) | -1 | -1 |
| G: -4242.91430 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10508.60459 HOMO: -6.81101 LUMO: -0.57960 factor:1 | 1 (-1.32460) | -1 | -1 |
| G: -4242.91430 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10508.65796 HOMO: -6.74298 LUMO: -0.57960 factor:1 | 1 (-1.37796) | -1 | -1 |
| G: -4242.91430 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10508.45520 HOMO: -6.63686 LUMO: -0.42994 factor:1 | 1 (-1.17521) | -1 | -1 |
| G: -4242.91430 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10508.65023 HOMO: -6.60965 LUMO: -0.41089 factor:1 | 1 (-1.37023) | -1 | -1 |
| G: -4242.91430 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10508.49567 HOMO: -6.60692 LUMO: -0.80274 factor:1 | 1 (-1.21567) | -1 | -1 |
| G: -4242.91430 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10508.64484 HOMO: -6.58788 LUMO: -0.78097 factor:1 | 1 (-1.36484) | -1 | -1 |
| G: -4242.91430 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10508.61496 HOMO: -6.67767 LUMO: -0.48436 factor:1 | 1 (-1.33496) | -1 | -1 |
| G: -4242.91430 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10508.77858 HOMO: -6.63141 LUMO: -0.40545 factor:1 | 1 (-1.49859) | -1 | -1 |
| G: -4242.91430 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10508.48212 HOMO: -6.62053 LUMO: -0.83811 factor:1 | 1 (-1.20212) | -1 | -1 |
| G: -4242.91430 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10508.98727 HOMO: -6.59604 LUMO: -0.35375 factor:1 | 1 (-1.70727) | -1 | -1 |
| G: -4242.91430 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10508.76574 HOMO: -6.34297 LUMO: -0.39729 factor:1 | 1 (-1.48574) | -1 | -1 |
| G: -4242.91430 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10507.92646 HOMO: -6.67223 LUMO: 1.97827 factor:1 | 1 (-0.64646) | -1 | -1 |
| G: -4242.91430 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10507.60183 HOMO: -6.40012 LUMO: 1.89935 factor:1 | 1 (-0.32183) | -1 | -1 |
| G: -4242.91430 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10507.47192 HOMO: -6.74842 LUMO: 1.97283 factor:1 | 1 (-0.19192) | -1 | -1 |
| G: -4242.91430 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10507.67206 HOMO: -6.76747 LUMO: 2.17147 factor:1 | 1 (-0.39206) | -1 | -1 |
| G: -4242.91430 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10507.81228 HOMO: -6.72121 LUMO: 1.55649 factor:1 | 1 (-0.53228) | -1 | -1 |
| G: -4242.91430 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10507.74986 HOMO: -6.97700 LUMO: 2.04085 factor:1 | 1 (-0.46986) | -1 | -1 |
| G: -4242.91430 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10507.57970 HOMO: -7.06680 LUMO: 2.04085 factor:1 | 1 (-0.29971) | 1 | 1 |
| G: -4242.91430 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10507.88624 HOMO: -7.09673 LUMO: 2.35106 factor:1 | 1 (-0.60624) | 1 | 1 |
| G: -4242.91430 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10507.68782 HOMO: -6.83006 LUMO: 2.14970 factor:1 | 1 (-0.40782) | -1 | -1 |
| G: -4242.91430 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10507.48479 HOMO: -6.72665 LUMO: 2.20140 factor:1 | 1 (-0.20479) | -1 | -1 |
| G: -4242.91430 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10507.25671 HOMO: -6.77291 LUMO: 2.34562 factor:1 | -1 (0.02329) | -1 | -1 |
| G: -4242.91430 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10507.57892 HOMO: -6.73754 LUMO: 2.00276 factor:1 | 1 (-0.29892) | -1 | -1 |
| G: -4242.91430 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10507.63848 HOMO: -7.04231 LUMO: 1.92112 factor:1 | 1 (-0.35848) | -1 | -1 |
| G: -4242.91430 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10507.82801 HOMO: -6.83822 LUMO: 1.72248 factor:1 | 1 (-0.54801) | -1 | -1 |
| G: -4242.91430 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10507.57911 HOMO: -6.57971 LUMO: 2.16603 factor:1 | 1 (-0.29911) | -1 | -1 |
| G: -4242.91430 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10507.72088 HOMO: -6.80013 LUMO: 1.88575 factor:1 | 1 (-0.44088) | -1 | -1 |
| G: -4242.91430 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10508.00935 HOMO: -6.93618 LUMO: 2.18235 factor:1 | 1 (-0.72935) | -1 | -1 |
| G: -4242.91430 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10507.54724 HOMO: -6.54706 LUMO: 1.91024 factor:1 | 1 (-0.26724) | -1 | -1 |
| G: -4242.91430 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10507.83002 HOMO: -7.06952 LUMO: 2.18507 factor:1 | 1 (-0.55002) | 1 | 1 |
| G: -4242.91430 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10507.83176 HOMO: -7.05047 LUMO: 1.82044 factor:1 | 1 (-0.55177) | -1 | -1 |
| G: -4242.91430 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10507.87228 HOMO: -6.87632 LUMO: 1.92657 factor:1 | 1 (-0.59228) | -1 | -1 |
| G: -4242.91430 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10507.60681 HOMO: -6.58788 LUMO: 1.91568 factor:1 | 1 (-0.32681) | -1 | -1 |
| G: -4242.91430 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10507.65554 HOMO: -7.17292 LUMO: 1.90752 factor:1 | 1 (-0.37554) | 1 | 1 |
| G: -4242.91430 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10507.88812 HOMO: -6.93890 LUMO: 1.80684 factor:1 | 1 (-0.60812) | -1 | -1 |
| G: -4242.91430 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10507.95900 HOMO: -7.10761 LUMO: 2.20956 factor:1 | 1 (-0.67901) | 1 | 1 |
| G: -4242.91430 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10507.48308 HOMO: -6.85727 LUMO: 2.13609 factor:1 | 1 (-0.20308) | -1 | -1 |
| G: -4242.91430 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10508.04722 HOMO: -6.64502 LUMO: 1.38506 factor:1 | 1 (-0.76723) | -1 | -1 |
| G: -4242.91430 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10507.95272 HOMO: -6.87360 LUMO: 1.15648 factor:1 | 1 (-0.67272) | -1 | -1 |
| G: -4242.91430 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10508.74041 HOMO: -6.67223 LUMO: 2.07351 factor:1 | 1 (-1.46041) | -1 | -1 |
| G: -4242.91430 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10508.49134 HOMO: -6.29671 LUMO: 2.43270 factor:1 | 1 (-1.21134) | -1 | -1 |
| G: -4242.91430 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10508.75197 HOMO: -6.90897 LUMO: 2.28848 factor:1 | 1 (-1.47197) | -1 | -1 |
| G: -4242.91430 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10508.79151 HOMO: -7.04231 LUMO: 1.70071 factor:1 | 1 (-1.51151) | -1 | -1 |
| G: -4242.91430 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10508.00589 HOMO: -6.69944 LUMO: 1.94834 factor:1 | 1 (-0.72589) | -1 | -1 |
| G: -4242.91430 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10507.44280 HOMO: -6.56067 LUMO: 2.20956 factor:1 | 1 (-0.16281) | -1 | -1 |
| G: -4242.91430 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10507.61492 HOMO: -6.65046 LUMO: 2.06807 factor:1 | 1 (-0.33492) | -1 | -1 |
| G: -4242.91430 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10507.72001 HOMO: -7.08584 LUMO: 1.98915 factor:1 | 1 (-0.44001) | 1 | 1 |
| G: -4242.91430 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10508.53052 HOMO: -6.69400 LUMO: 2.09256 factor:1 | 1 (-1.25053) | -1 | -1 |
| G: -4242.91430 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10508.69983 HOMO: -6.62869 LUMO: 2.16331 factor:1 | 1 (-1.41984) | -1 | -1 |
| G: -4242.91430 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10508.54576 HOMO: -6.85183 LUMO: 2.16058 factor:1 | 1 (-1.26576) | -1 | -1 |
| G: -4242.91430 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10508.58321 HOMO: -6.54706 LUMO: 1.92384 factor:1 | 1 (-1.30321) | -1 | -1 |
| G: -4242.91430 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10508.81429 HOMO: -6.84366 LUMO: 2.48984 factor:1 | 1 (-1.53429) | -1 | -1 |
| G: -4242.91430 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10508.81146 HOMO: -6.77291 LUMO: 2.46263 factor:1 | 1 (-1.53146) | -1 | -1 |
| G: -4242.91430 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10508.60917 HOMO: -7.01782 LUMO: 2.31025 factor:1 | 1 (-1.32917) | -1 | -1 |
| G: -4242.91430 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10508.69159 HOMO: -6.94707 LUMO: 2.29664 factor:1 | 1 (-1.41159) | -1 | -1 |
| G: -4242.91430 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10508.36064 HOMO: -6.64230 LUMO: 1.97283 factor:1 | 1 (-1.08065) | -1 | -1 |
| G: -4242.91430 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10508.32331 HOMO: -6.47359 LUMO: 2.20412 factor:1 | 1 (-1.04331) | -1 | -1 |
| G: -4242.91430 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10508.53833 HOMO: -6.90625 LUMO: 1.92384 factor:1 | 1 (-1.25834) | -1 | -1 |
| G: -4242.91430 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10507.64847 HOMO: -7.17020 LUMO: 2.06807 factor:1 | 1 (-0.36847) | 1 | 1 |
| G: -4242.91430 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10507.62814 HOMO: -6.65046 LUMO: 2.20956 factor:1 | 1 (-0.34814) | -1 | -1 |
| G: -4242.91430 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10507.81288 HOMO: -7.07496 LUMO: 1.82861 factor:1 | 1 (-0.53288) | 1 | 1 |
| G: -4242.91430 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10507.54177 HOMO: -6.83006 LUMO: 2.14970 factor:1 | 1 (-0.26177) | -1 | -1 |
| G: -4242.91430 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10507.83171 HOMO: -6.92802 LUMO: 1.99187 factor:1 | 1 (-0.55171) | -1 | -1 |
| G: -4242.91430 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10507.60085 HOMO: -6.69672 LUMO: 2.36739 factor:1 | 1 (-0.32085) | -1 | -1 |
| G: -4242.91430 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10507.83130 HOMO: -7.13755 LUMO: 2.00276 factor:1 | 1 (-0.55130) | 1 | 1 |
| G: -4242.91430 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10507.69165 HOMO: -6.92530 LUMO: 2.25582 factor:1 | 1 (-0.41165) | -1 | -1 |
| G: -4242.91430 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10507.79092 HOMO: -6.77564 LUMO: 1.97827 factor:1 | 1 (-0.51092) | -1 | -1 |
| G: -4242.91430 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10507.79073 HOMO: -6.87904 LUMO: 1.60003 factor:1 | 1 (-0.51073) | -1 | -1 |
| G: -4242.91430 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10507.94200 HOMO: -6.62869 LUMO: 1.90480 factor:1 | 1 (-0.66200) | -1 | -1 |
| G: -4242.91430 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10508.04839 HOMO: -6.71033 LUMO: 1.54833 factor:1 | 1 (-0.76840) | -1 | -1 |
| G: -4242.91430 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10508.08429 HOMO: -6.74298 LUMO: 1.47486 factor:1 | 1 (-0.80429) | -1 | -1 |
| G: -4242.91430 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10507.80964 HOMO: -6.77019 LUMO: 1.90480 factor:1 | 1 (-0.52964) | -1 | -1 |
| G: -4242.91430 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -10507.74526 HOMO: -6.70489 LUMO: 1.99459 factor:1 | 1 (-0.46526) | -1 | -1 |