乙二醇作为反应物的反应表19-12

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: -6289.33611 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.29114 HOMO: -6.91169 LUMO: -0.53879 factor:1 | 1 (-1.58934) | -1 | -1 |
| G: -6289.33611 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.09334 HOMO: -7.29809 LUMO: 2.83543 factor:1 | 1 (-1.39154) | 1 | -1 |
| G: -6289.33611 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.70125 HOMO: -6.86543 LUMO: -0.70205 factor:1 | 1 (-1.99944) | -1 | -1 |
| G: -6289.33611 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.47221 HOMO: -7.47769 LUMO: 0.31293 factor:1 | 1 (-1.77040) | -1 | -1 |
| G: -6289.33611 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.67575 HOMO: -6.63141 LUMO: -0.55511 factor:1 | 1 (-1.97394) | -1 | -1 |
| G: -6289.33611 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12556.24724 HOMO: -6.68856 LUMO: -0.30205 factor:1 | 1 (-2.54543) | -1 | -1 |
| G: -6289.33611 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.42998 HOMO: -7.22190 LUMO: 0.53334 factor:1 | 1 (-1.72817) | -1 | -1 |
| G: -6289.33611 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12556.02416 HOMO: -6.66407 LUMO: -0.27756 factor:1 | 1 (-2.32236) | -1 | -1 |
| G: -6289.33611 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.28502 HOMO: -7.15659 LUMO: -0.70205 factor:1 | 1 (-1.58321) | -1 | -1 |
| G: -6289.33611 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.44636 HOMO: -6.69400 LUMO: 1.67622 factor:1 | 1 (-1.74455) | -1 | -1 |
| G: -6289.33611 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.29955 HOMO: -6.60420 LUMO: 2.16058 factor:1 | 1 (-1.59774) | -1 | -1 |
| G: -6289.33611 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.13996 HOMO: -6.87087 LUMO: 1.88031 factor:1 | 1 (-1.43815) | -1 | -1 |
| G: -6289.33611 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.45069 HOMO: -6.60965 LUMO: -0.19864 factor:1 | 1 (-0.74888) | -1 | -1 |
| G: -6289.33611 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.28729 HOMO: -7.29265 LUMO: 0.52246 factor:1 | 1 (-0.58548) | -1 | -1 |
| G: -6289.33611 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.28609 HOMO: -6.86543 LUMO: -0.59593 factor:1 | 1 (-0.58428) | -1 | -1 |
| G: -6289.33611 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.41619 HOMO: -7.44504 LUMO: -1.01226 factor:1 | 1 (-0.71438) | -1 | -1 |
| G: -6289.33611 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.45989 HOMO: -6.92530 LUMO: -0.75103 factor:1 | 1 (-0.75808) | -1 | -1 |
| G: -6289.33611 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.17227 HOMO: -7.10489 LUMO: 2.20412 factor:1 | 1 (-0.47046) | 1 | 1 |
| G: -6289.33611 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.18378 HOMO: -6.58788 LUMO: 1.73881 factor:1 | 1 (-0.48197) | -1 | -1 |
| G: -6289.33611 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.42408 HOMO: -6.64502 LUMO: 1.70343 factor:1 | 1 (-0.72227) | -1 | -1 |
| G: -6289.33611 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.23956 HOMO: -6.73754 LUMO: 1.60819 factor:1 | 1 (-0.53775) | -1 | -1 |
| G: -6289.33611 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.01452 HOMO: -6.80829 LUMO: 2.45991 factor:1 | 1 (-0.31271) | -1 | -1 |
| G: -6289.33611 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.36002 HOMO: -6.91713 LUMO: 2.43814 factor:1 | 1 (-0.65822) | -1 | -1 |
| G: -6289.33611 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.24974 HOMO: -6.60692 LUMO: 1.93745 factor:1 | 1 (-0.54793) | -1 | -1 |
| G: -6289.33611 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.69458 HOMO: -6.26134 LUMO: 1.46125 factor:1 | 1 (-1.99277) | -1 | -1 |
| G: -6289.33611 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12556.54091 HOMO: -7.54028 LUMO: 0.25851 factor:1 | 1 (-2.83910) | -1 | -1 |
| G: -6289.33611 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.47561 HOMO: -6.97700 LUMO: -0.73471 factor:1 | 1 (-1.77380) | -1 | -1 |
| G: -6289.33611 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.17578 HOMO: -6.92258 LUMO: -0.70205 factor:1 | 1 (-0.47397) | -1 | -1 |
| G: -6289.33611 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.32821 HOMO: -6.83550 LUMO: -0.56872 factor:1 | 1 (-0.62641) | -1 | -1 |
| G: -6289.33611 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.30291 HOMO: -6.72121 LUMO: 1.89663 factor:1 | 1 (-0.60110) | -1 | -1 |
| G: -6289.33611 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.90936 HOMO: -6.73482 LUMO: 1.89935 factor:1 | 1 (-2.20755) | -1 | -1 |
| G: -6289.33611 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.22799 HOMO: -6.61781 LUMO: 1.86670 factor:1 | 1 (-1.52618) | -1 | -1 |
| G: -6289.33611 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.76027 HOMO: -7.01782 LUMO: 2.26399 factor:1 | 1 (-2.05846) | -1 | -1 |
| G: -6289.33611 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.15008 HOMO: -7.23551 LUMO: 2.09800 factor:1 | 1 (-1.44827) | 1 | 1 |
| G: -6289.33611 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.30859 HOMO: -7.13483 LUMO: 2.17963 factor:1 | 1 (-1.60678) | 1 | 1 |
| G: -6289.33611 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12556.02985 HOMO: -6.22869 LUMO: 2.01092 factor:1 | 1 (-2.32804) | -1 | -1 |
| G: -6289.33611 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.39613 HOMO: -6.80285 LUMO: 2.14970 factor:1 | 1 (-1.69432) | -1 | -1 |
| G: -6289.33611 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12556.18607 HOMO: -7.21102 LUMO: 2.33746 factor:1 | 1 (-2.48426) | 1 | 1 |
| G: -6289.33611 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.23756 HOMO: -6.39740 LUMO: 2.59597 factor:1 | 1 (-1.53576) | -1 | -1 |
| G: -6289.33611 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.66379 HOMO: -7.07768 LUMO: 2.48168 factor:1 | 1 (-0.96198) | 1 | 1 |
| G: -6289.33611 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.52811 HOMO: -7.11306 LUMO: 0.90614 factor:1 | 1 (-0.82630) | -1 | -1 |
| G: -6289.33611 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.71554 HOMO: -6.61781 LUMO: -2.46263 factor:1 | 1 (-1.01373) | -1 | -1 |
| G: -6289.33611 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.53162 HOMO: -6.96611 LUMO: 0.90614 factor:1 | 1 (-0.82981) | -1 | -1 |
| G: -6289.33611 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.36748 HOMO: -6.86271 LUMO: -1.14832 factor:1 | 1 (-0.66567) | -1 | -1 |
| G: -6289.33611 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.70226 HOMO: -6.72665 LUMO: 0.96873 factor:1 | 1 (-1.00045) | -1 | -1 |
| G: -6289.33611 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.97987 HOMO: -7.14571 LUMO: 1.05036 factor:1 | 1 (-1.27806) | -1 | -1 |
| G: -6289.33611 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.93024 HOMO: -7.14299 LUMO: 0.98777 factor:1 | 1 (-1.22843) | -1 | -1 |
| G: -6289.33611 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.80942 HOMO: -6.99333 LUMO: 1.05852 factor:1 | 1 (-1.10761) | -1 | -1 |
| G: -6289.33611 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.43570 HOMO: -6.78924 LUMO: -1.49935 factor:1 | 1 (-0.73389) | -1 | -1 |
| G: -6289.33611 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.96667 HOMO: -7.13755 LUMO: 0.94151 factor:1 | 1 (-1.26487) | -1 | -1 |
| G: -6289.33611 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.70354 HOMO: -6.72938 LUMO: -0.35375 factor:1 | 1 (-1.00173) | -1 | -1 |
| G: -6289.33611 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.84681 HOMO: -6.99061 LUMO: 0.82450 factor:1 | 1 (-1.14500) | -1 | -1 |
| G: -6289.33611 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.75056 HOMO: -6.75114 LUMO: -0.68028 factor:1 | 1 (-1.04875) | -1 | -1 |
| G: -6289.33611 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.85497 HOMO: -6.40556 LUMO: -0.42722 factor:1 | 1 (-1.15316) | -1 | -1 |
| G: -6289.33611 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.87220 HOMO: -7.18653 LUMO: 0.42178 factor:1 | 1 (-1.17039) | -1 | -1 |
| G: -6289.33611 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.69236 HOMO: -6.63958 LUMO: -0.71294 factor:1 | 1 (-0.99055) | -1 | -1 |
| G: -6289.33611 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.53344 HOMO: -6.63958 LUMO: -0.71022 factor:1 | 1 (-0.83163) | -1 | -1 |
| G: -6289.33611 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.70104 HOMO: -6.69672 LUMO: -0.72654 factor:1 | 1 (-0.99923) | -1 | -1 |
| G: -6289.33611 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.68400 HOMO: -6.56883 LUMO: -0.80274 factor:1 | 1 (-0.98219) | -1 | -1 |
| G: -6289.33611 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.37143 HOMO: -6.68584 LUMO: -0.56872 factor:1 | 1 (-0.66962) | -1 | -1 |
| G: -6289.33611 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.71546 HOMO: -6.59060 LUMO: -0.35647 factor:1 | 1 (-1.01365) | -1 | -1 |
| G: -6289.33611 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.74888 HOMO: -6.72121 LUMO: -0.71838 factor:1 | 1 (-1.04707) | -1 | -1 |
| G: -6289.33611 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.37329 HOMO: -6.57971 LUMO: -0.61498 factor:1 | 1 (-1.67149) | -1 | -1 |
| G: -6289.33611 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.41319 HOMO: -7.07496 LUMO: 0.50613 factor:1 | 1 (-1.71138) | -1 | -1 |
| G: -6289.33611 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.61496 HOMO: -7.14027 LUMO: 0.43266 factor:1 | 1 (-1.91315) | -1 | -1 |
| G: -6289.33611 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.59529 HOMO: -6.43277 LUMO: -0.44082 factor:1 | 1 (-1.89348) | -1 | -1 |
| G: -6289.33611 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.52426 HOMO: -6.79468 LUMO: 0.07619 factor:1 | 1 (-1.82246) | -1 | -1 |
| G: -6289.33611 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.46176 HOMO: -6.81917 LUMO: -2.57148 factor:1 | 1 (-1.75995) | -1 | -1 |
| G: -6289.33611 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.80063 HOMO: -6.71849 LUMO: 1.30615 factor:1 | 1 (-1.09882) | -1 | -1 |
| G: -6289.33611 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.93165 HOMO: -6.85455 LUMO: -0.63675 factor:1 | 1 (-1.22985) | -1 | -1 |
| G: -6289.33611 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.79171 HOMO: -6.73210 LUMO: -1.03131 factor:1 | 1 (-1.08990) | -1 | -1 |
| G: -6289.33611 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.04488 HOMO: -6.83550 LUMO: -0.58777 factor:1 | 1 (-1.34307) | -1 | -1 |
| G: -6289.33611 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.32366 HOMO: -6.53073 LUMO: -0.74287 factor:1 | 1 (-1.62185) | -1 | -1 |
| G: -6289.33611 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.24480 HOMO: -7.18381 LUMO: -0.92791 factor:1 | 1 (-1.54299) | -1 | -1 |
| G: -6289.33611 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.30709 HOMO: -6.49264 LUMO: -0.44627 factor:1 | 1 (-1.60528) | -1 | -1 |
| G: -6289.33611 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.36823 HOMO: -7.32803 LUMO: 0.41361 factor:1 | 1 (-1.66643) | -1 | -1 |
| G: -6289.33611 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.25479 HOMO: -6.53073 LUMO: -0.52790 factor:1 | 1 (-1.55298) | -1 | -1 |
| G: -6289.33611 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.98858 HOMO: -6.54978 LUMO: -0.53062 factor:1 | 1 (-1.28677) | -1 | -1 |
| G: -6289.33611 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.49531 HOMO: -6.56611 LUMO: -0.37824 factor:1 | 1 (-1.79350) | -1 | -1 |
| G: -6289.33611 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.42979 HOMO: -6.57155 LUMO: -0.64219 factor:1 | 1 (-1.72798) | -1 | -1 |
| G: -6289.33611 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.28491 HOMO: -7.08040 LUMO: 0.45715 factor:1 | 1 (-1.58310) | -1 | -1 |
| G: -6289.33611 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.09043 HOMO: -6.66679 LUMO: -0.75376 factor:1 | 1 (-1.38862) | -1 | -1 |
| G: -6289.33611 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.10589 HOMO: -6.83550 LUMO: -0.99322 factor:1 | 1 (-1.40408) | -1 | -1 |
| G: -6289.33611 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.33610 HOMO: -6.53345 LUMO: -0.29660 factor:1 | 1 (-1.63429) | -1 | -1 |
| G: -6289.33611 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.36807 HOMO: -6.65046 LUMO: 2.40549 factor:1 | 1 (-1.66626) | -1 | -1 |
| G: -6289.33611 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.10679 HOMO: -6.98788 LUMO: 2.01092 factor:1 | 1 (-1.40498) | -1 | -1 |
| G: -6289.33611 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.94224 HOMO: -6.61781 LUMO: 1.92384 factor:1 | 1 (-1.24043) | -1 | -1 |
| G: -6289.33611 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.29370 HOMO: -6.61237 LUMO: 2.06807 factor:1 | 1 (-1.59189) | -1 | -1 |
| G: -6289.33611 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.35142 HOMO: -6.59060 LUMO: 1.95106 factor:1 | 1 (-1.64961) | -1 | -1 |
| G: -6289.33611 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.63042 HOMO: -6.48175 LUMO: 1.72248 factor:1 | 1 (-0.92862) | -1 | -1 |
| G: -6289.33611 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.56806 HOMO: -6.84911 LUMO: 2.03541 factor:1 | 1 (-0.86625) | -1 | -1 |
| G: -6289.33611 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.39341 HOMO: -6.50624 LUMO: 2.17147 factor:1 | 1 (-0.69160) | -1 | -1 |
| G: -6289.33611 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.21458 HOMO: -6.68312 LUMO: 2.08439 factor:1 | 1 (-0.51277) | -1 | -1 |
| G: -6289.33611 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.14043 HOMO: -6.96067 LUMO: 1.98099 factor:1 | 1 (-0.43862) | -1 | -1 |
| G: -6289.33611 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.77296 HOMO: -6.93618 LUMO: 1.85854 factor:1 | 1 (-1.07115) | -1 | -1 |
| G: -6289.33611 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.45850 HOMO: -6.71305 LUMO: -0.61226 factor:1 | 1 (-0.75669) | -1 | -1 |
| G: -6289.33611 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.61687 HOMO: -7.06408 LUMO: 0.80001 factor:1 | 1 (-0.91506) | -1 | -1 |
| G: -6289.33611 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.70006 HOMO: -6.52257 LUMO: 0.99049 factor:1 | 1 (-0.99825) | -1 | -1 |
| G: -6289.33611 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.50748 HOMO: -6.84638 LUMO: 1.10750 factor:1 | 1 (-0.80567) | -1 | -1 |
| G: -6289.33611 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.34389 HOMO: -6.85455 LUMO: 0.84900 factor:1 | 1 (-0.64208) | -1 | -1 |
| G: -6289.33611 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.59108 HOMO: -6.60148 LUMO: -0.78369 factor:1 | 1 (-0.88927) | -1 | -1 |
| G: -6289.33611 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.49173 HOMO: -6.86543 LUMO: -0.93063 factor:1 | 1 (-0.78992) | -1 | -1 |
| G: -6289.33611 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.62348 HOMO: -6.70489 LUMO: -0.72382 factor:1 | 1 (-0.92168) | -1 | -1 |
| G: -6289.33611 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.41907 HOMO: -6.59060 LUMO: 0.31293 factor:1 | 1 (-0.71726) | -1 | -1 |
| G: -6289.33611 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.27417 HOMO: -6.52257 LUMO: -0.48708 factor:1 | 1 (-0.57236) | -1 | -1 |
| G: -6289.33611 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.55823 HOMO: -6.54706 LUMO: -0.48164 factor:1 | 1 (-0.85642) | -1 | -1 |
| G: -6289.33611 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.24412 HOMO: -7.32803 LUMO: 0.08436 factor:1 | 1 (-1.54231) | -1 | -1 |
| G: -6289.33611 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.28050 HOMO: -6.77291 LUMO: -0.66940 factor:1 | 1 (-1.57870) | -1 | -1 |
| G: -6289.33611 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.20548 HOMO: -6.68312 LUMO: -0.53062 factor:1 | 1 (-1.50367) | -1 | -1 |
| G: -6289.33611 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.85255 HOMO: -7.07768 LUMO: 0.45987 factor:1 | 1 (-1.15074) | -1 | -1 |
| G: -6289.33611 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.27327 HOMO: -6.50352 LUMO: -0.63675 factor:1 | 1 (-1.57146) | -1 | -1 |
| G: -6289.33611 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.07533 HOMO: -6.48992 LUMO: -0.60681 factor:1 | 1 (-1.37352) | -1 | -1 |
| G: -6289.33611 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.75056 HOMO: -6.65318 LUMO: -0.72382 factor:1 | 1 (-1.04875) | -1 | -1 |
| G: -6289.33611 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.52359 HOMO: -6.54706 LUMO: 0.24218 factor:1 | 1 (-0.82178) | -1 | -1 |
| G: -6289.33611 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.60291 HOMO: -6.63958 LUMO: 0.57416 factor:1 | 1 (-0.90111) | -1 | -1 |
| G: -6289.33611 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.25371 HOMO: -6.37563 LUMO: -0.48164 factor:1 | 1 (-0.55190) | -1 | -1 |
| G: -6289.33611 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.67540 HOMO: -6.64774 LUMO: -0.71838 factor:1 | 1 (-0.97360) | -1 | -1 |
| G: -6289.33611 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.34794 HOMO: -7.17020 LUMO: 0.45987 factor:1 | 1 (-0.64613) | -1 | -1 |
| G: -6289.33611 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.19618 HOMO: -6.86543 LUMO: -1.05036 factor:1 | 1 (-0.49438) | -1 | -1 |
| G: -6289.33611 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.47156 HOMO: -6.77019 LUMO: -1.03131 factor:1 | 1 (-0.76976) | -1 | -1 |
| G: -6289.33611 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.44552 HOMO: -6.80285 LUMO: 1.05852 factor:1 | 1 (-0.74371) | -1 | -1 |
| G: -6289.33611 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.63059 HOMO: -6.76475 LUMO: 1.01771 factor:1 | 1 (-0.92878) | -1 | -1 |
| G: -6289.33611 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.74634 HOMO: -6.92530 LUMO: 1.37417 factor:1 | 1 (-1.04454) | -1 | -1 |
| G: -6289.33611 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.83247 HOMO: -6.98244 LUMO: 1.25989 factor:1 | 1 (-1.13066) | -1 | -1 |
| G: -6289.33611 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.58528 HOMO: -6.74842 LUMO: 0.89798 factor:1 | 1 (-0.88347) | -1 | -1 |
| G: -6289.33611 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.54672 HOMO: -6.77019 LUMO: -1.17009 factor:1 | 1 (-0.84491) | -1 | -1 |
| G: -6289.33611 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.42247 HOMO: -6.78652 LUMO: 1.35785 factor:1 | 1 (-0.72067) | -1 | -1 |
| G: -6289.33611 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.54158 HOMO: -6.82734 LUMO: -0.68301 factor:1 | 1 (-0.83977) | -1 | -1 |
| G: -6289.33611 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.55548 HOMO: -6.48175 LUMO: -2.19052 factor:1 | 1 (-0.85368) | -1 | -1 |
| G: -6289.33611 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.29717 HOMO: -6.65863 LUMO: -0.77008 factor:1 | 1 (-0.59536) | -1 | -1 |
| G: -6289.33611 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.61508 HOMO: -6.44094 LUMO: -2.20956 factor:1 | 1 (-0.91327) | -1 | -1 |
| G: -6289.33611 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.26838 HOMO: -6.59876 LUMO: -0.57688 factor:1 | 1 (-0.56657) | -1 | -1 |
| G: -6289.33611 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.37134 HOMO: -6.78380 LUMO: -0.77008 factor:1 | 1 (-0.66954) | -1 | -1 |
| G: -6289.33611 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.18625 HOMO: -7.30354 LUMO: 0.25034 factor:1 | 1 (-0.48444) | -1 | -1 |
| G: -6289.33611 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.00451 HOMO: -6.59332 LUMO: -0.53334 factor:1 | 1 (-0.30270) | -1 | -1 |
| G: -6289.33611 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.50678 HOMO: -6.64230 LUMO: -0.55783 factor:1 | 1 (-0.80497) | -1 | -1 |
| G: -6289.33611 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.17507 HOMO: -7.26544 LUMO: 0.20409 factor:1 | 1 (-0.47326) | -1 | -1 |
| G: -6289.33611 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.76575 HOMO: -6.61237 LUMO: -0.65307 factor:1 | 1 (-1.06394) | -1 | -1 |
| G: -6289.33611 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.65780 HOMO: -6.72393 LUMO: -0.65307 factor:1 | 1 (-0.95599) | -1 | -1 |
| G: -6289.33611 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.14975 HOMO: -6.29671 LUMO: -0.39729 factor:1 | 1 (-1.44795) | -1 | -1 |
| G: -6289.33611 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.18023 HOMO: -6.75387 LUMO: -0.53334 factor:1 | 1 (-1.47842) | -1 | -1 |
| G: -6289.33611 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.04140 HOMO: -6.53073 LUMO: -0.31293 factor:1 | 1 (-1.33959) | -1 | -1 |
| G: -6289.33611 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.36113 HOMO: -6.42189 LUMO: -0.59049 factor:1 | 1 (-1.65932) | -1 | -1 |
| G: -6289.33611 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.41039 HOMO: -6.41100 LUMO: -0.29933 factor:1 | 1 (-0.70858) | -1 | -1 |
| G: -6289.33611 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.26166 HOMO: -6.57427 LUMO: -0.53879 factor:1 | 1 (-0.55985) | -1 | -1 |
| G: -6289.33611 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12553.97194 HOMO: -7.43143 LUMO: 0.33470 factor:1 | 1 (-0.27013) | -1 | -1 |
| G: -6289.33611 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.07330 HOMO: -6.56067 LUMO: -0.50885 factor:1 | 1 (-0.37149) | -1 | -1 |
| G: -6289.33611 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12553.76902 HOMO: -6.65863 LUMO: -0.76464 factor:1 | 1 (-0.06721) | -1 | -1 |
| G: -6289.33611 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12553.41067 HOMO: -6.32665 LUMO: -0.41906 factor:1 | -1 (0.29113) | -1 | -1 |
| G: -6289.33611 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.17548 HOMO: -6.57699 LUMO: 1.63813 factor:1 | 1 (-0.47367) | -1 | -1 |
| G: -6289.33611 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.85171 HOMO: -6.53073 LUMO: 1.71704 factor:1 | 1 (-1.14990) | -1 | -1 |
| G: -6289.33611 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.72523 HOMO: -6.86271 LUMO: 2.07351 factor:1 | 1 (-1.02342) | -1 | -1 |
| G: -6289.33611 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.63233 HOMO: -6.63686 LUMO: 1.78235 factor:1 | 1 (-0.93052) | -1 | -1 |
| G: -6289.33611 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.82349 HOMO: -6.60965 LUMO: 1.94289 factor:1 | 1 (-1.12168) | -1 | -1 |
| G: -6289.33611 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.54321 HOMO: -6.55250 LUMO: 1.89119 factor:1 | 1 (-0.84140) | -1 | -1 |
| G: -6289.33611 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.64433 HOMO: -6.50624 LUMO: 1.85582 factor:1 | 1 (-0.94252) | -1 | -1 |
| G: -6289.33611 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.39890 HOMO: -6.06814 LUMO: 1.94561 factor:1 | 1 (-1.69709) | -1 | -1 |
| G: -6289.33611 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.51724 HOMO: -6.58788 LUMO: 2.01908 factor:1 | 1 (-1.81543) | -1 | -1 |
| G: -6289.33611 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.55733 HOMO: -6.74026 LUMO: 0.31293 factor:1 | 1 (-1.85552) | -1 | -1 |
| G: -6289.33611 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.30592 HOMO: -6.54434 LUMO: -0.42994 factor:1 | 1 (-1.60411) | -1 | -1 |
| G: -6289.33611 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.35501 HOMO: -6.94707 LUMO: 0.42994 factor:1 | 1 (-1.65320) | -1 | -1 |
| G: -6289.33611 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.73402 HOMO: -6.98516 LUMO: 0.41361 factor:1 | 1 (-1.03221) | -1 | -1 |
| G: -6289.33611 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.80036 HOMO: -6.31304 LUMO: -0.54967 factor:1 | 1 (-1.09855) | -1 | -1 |
| G: -6289.33611 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.63363 HOMO: -6.48447 LUMO: -0.40817 factor:1 | 1 (-0.93183) | -1 | -1 |
| G: -6289.33611 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.52204 HOMO: -6.49264 LUMO: 0.29116 factor:1 | 1 (-0.82023) | -1 | -1 |
| G: -6289.33611 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.42841 HOMO: -6.48719 LUMO: -0.11973 factor:1 | 1 (-0.72660) | -1 | -1 |
| G: -6289.33611 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.35205 HOMO: -7.16204 LUMO: 0.44082 factor:1 | 1 (-0.65024) | -1 | -1 |
| G: -6289.33611 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.38996 HOMO: -6.74842 LUMO: -0.37552 factor:1 | 1 (-0.68815) | -1 | -1 |
| G: -6289.33611 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.11594 HOMO: -6.44638 LUMO: -0.45171 factor:1 | 1 (-0.41413) | -1 | -1 |
| G: -6289.33611 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.48307 HOMO: -7.07496 LUMO: 0.50341 factor:1 | 1 (-0.78127) | -1 | -1 |
| G: -6289.33611 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.35400 HOMO: -6.79468 LUMO: 0.11429 factor:1 | 1 (-1.65219) | -1 | -1 |
| G: -6289.33611 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.54952 HOMO: -6.63958 LUMO: -0.67484 factor:1 | 1 (-1.84771) | -1 | -1 |
| G: -6289.33611 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.08924 HOMO: -7.08584 LUMO: 0.46259 factor:1 | 1 (-1.38743) | -1 | -1 |
| G: -6289.33611 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.51860 HOMO: -6.80285 LUMO: -0.73199 factor:1 | 1 (-1.81680) | -1 | -1 |
| G: -6289.33611 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.36355 HOMO: -6.44366 LUMO: -0.45443 factor:1 | 1 (-1.66174) | -1 | -1 |
| G: -6289.33611 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.80575 HOMO: -6.75931 LUMO: 0.25851 factor:1 | 1 (-1.10394) | -1 | -1 |
| G: -6289.33611 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.54626 HOMO: -6.64502 LUMO: 1.79323 factor:1 | 1 (-0.84445) | -1 | -1 |
| G: -6289.33611 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.68245 HOMO: -6.51168 LUMO: 1.60275 factor:1 | 1 (-0.98064) | -1 | -1 |
| G: -6289.33611 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.37311 HOMO: -6.56067 LUMO: 1.63268 factor:1 | 1 (-0.67130) | -1 | -1 |
| G: -6289.33611 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.17839 HOMO: -6.56883 LUMO: 1.70615 factor:1 | 1 (-0.47658) | -1 | -1 |
| G: -6289.33611 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.39826 HOMO: -6.77836 LUMO: 1.77962 factor:1 | 1 (-0.69645) | -1 | -1 |
| G: -6289.33611 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.60539 HOMO: -6.38923 LUMO: 1.85854 factor:1 | 1 (-0.90358) | -1 | -1 |
| G: -6289.33611 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.75625 HOMO: -6.35658 LUMO: 2.16875 factor:1 | 1 (-1.05444) | -1 | -1 |
| G: -6289.33611 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.44792 HOMO: -6.83006 LUMO: 2.31025 factor:1 | 1 (-0.74611) | -1 | -1 |
| G: -6289.33611 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.55932 HOMO: -6.87087 LUMO: 1.79051 factor:1 | 1 (-0.85751) | -1 | -1 |
| G: -6289.33611 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.62261 HOMO: -6.56339 LUMO: 2.37828 factor:1 | 1 (-0.92081) | -1 | -1 |
| G: -6289.33611 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.19605 HOMO: -6.30488 LUMO: 2.51705 factor:1 | 1 (-0.49424) | -1 | -1 |
| G: -6289.33611 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.19891 HOMO: -6.69400 LUMO: 1.95650 factor:1 | 1 (-0.49710) | -1 | -1 |
| G: -6289.33611 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12553.93044 HOMO: -6.51168 LUMO: 2.03541 factor:1 | 1 (-0.22863) | -1 | -1 |
| G: -6289.33611 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.33929 HOMO: -6.30760 LUMO: 1.65173 factor:1 | 1 (-0.63748) | -1 | -1 |
| G: -6289.33611 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.55102 HOMO: -6.55250 LUMO: 1.90752 factor:1 | 1 (-0.84921) | -1 | -1 |
| G: -6289.33611 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.54346 HOMO: -6.41372 LUMO: 1.76058 factor:1 | 1 (-0.84165) | -1 | -1 |
| G: -6289.33611 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.52451 HOMO: -6.23957 LUMO: 2.06534 factor:1 | 1 (-1.82270) | -1 | -1 |
| G: -6289.33611 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.58799 HOMO: -6.58243 LUMO: 2.11705 factor:1 | 1 (-1.88618) | -1 | -1 |
| G: -6289.33611 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.34230 HOMO: -6.37835 LUMO: 2.09256 factor:1 | 1 (-1.64049) | -1 | -1 |
| G: -6289.33611 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.37732 HOMO: -6.50624 LUMO: 2.55787 factor:1 | 1 (-1.67551) | -1 | -1 |
| G: -6289.33611 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.20799 HOMO: -6.45454 LUMO: 1.87214 factor:1 | 1 (-1.50618) | -1 | -1 |
| G: -6289.33611 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.24102 HOMO: -6.53617 LUMO: 1.95650 factor:1 | 1 (-1.53921) | -1 | -1 |
| G: -6289.33611 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.19558 HOMO: -6.51985 LUMO: 1.71432 factor:1 | 1 (-1.49377) | -1 | -1 |
| G: -6289.33611 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.38140 HOMO: -6.75114 LUMO: 1.84493 factor:1 | 1 (-1.67960) | -1 | -1 |
| G: -6289.33611 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.28284 HOMO: -6.06270 LUMO: 1.65717 factor:1 | 1 (-1.58104) | -1 | -1 |
| G: -6289.33611 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.01748 HOMO: -5.89671 LUMO: 1.71704 factor:1 | 1 (-1.31567) | -1 | -1 |
| G: -6289.33611 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.35865 HOMO: -6.18787 LUMO: 1.91840 factor:1 | 1 (-1.65685) | -1 | -1 |
| G: -6289.33611 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.25729 HOMO: -6.01644 LUMO: 1.85582 factor:1 | 1 (-1.55548) | -1 | -1 |
| G: -6289.33611 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.27884 HOMO: -6.05998 LUMO: 2.33474 factor:1 | 1 (-1.57704) | -1 | -1 |
| G: -6289.33611 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.10858 HOMO: -6.05725 LUMO: 2.03541 factor:1 | 1 (-1.40677) | -1 | -1 |
| G: -6289.33611 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.32355 HOMO: -6.80829 LUMO: 1.90480 factor:1 | 1 (-1.62174) | -1 | -1 |
| G: -6289.33611 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.35972 HOMO: -6.76475 LUMO: 2.20956 factor:1 | 1 (-1.65791) | -1 | -1 |
| G: -6289.33611 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.51466 HOMO: -6.29944 LUMO: 1.77962 factor:1 | 1 (-1.81285) | -1 | -1 |
| G: -6289.33611 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.34935 HOMO: -6.47359 LUMO: -0.25579 factor:1 | 1 (-1.64754) | -1 | -1 |
| G: -6289.33611 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.16924 HOMO: -6.57699 LUMO: -0.47348 factor:1 | 1 (-1.46743) | -1 | -1 |
| G: -6289.33611 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.10091 HOMO: -7.20830 LUMO: 0.49797 factor:1 | 1 (-1.39910) | -1 | -1 |
| G: -6289.33611 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.39294 HOMO: -7.49402 LUMO: 0.29933 factor:1 | 1 (-1.69113) | -1 | -1 |
| G: -6289.33611 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.40271 HOMO: -6.66679 LUMO: -0.58777 factor:1 | 1 (-1.70090) | -1 | -1 |
| G: -6289.33611 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.43825 HOMO: -6.67767 LUMO: -0.56328 factor:1 | 1 (-1.73644) | -1 | -1 |
| G: -6289.33611 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.23220 HOMO: -7.42871 LUMO: 0.35647 factor:1 | 1 (-1.53040) | -1 | -1 |
| G: -6289.33611 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.40211 HOMO: -6.56067 LUMO: -0.54423 factor:1 | 1 (-1.70030) | -1 | -1 |
| G: -6289.33611 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.02986 HOMO: -6.56339 LUMO: -0.50341 factor:1 | 1 (-1.32805) | -1 | -1 |
| G: -6289.33611 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.99214 HOMO: -6.56067 LUMO: -0.48436 factor:1 | 1 (-1.29034) | -1 | -1 |
| G: -6289.33611 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.32070 HOMO: -6.73210 LUMO: 1.75241 factor:1 | 1 (-1.61889) | -1 | -1 |
| G: -6289.33611 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.17234 HOMO: -6.48175 LUMO: 1.91296 factor:1 | 1 (-1.47053) | -1 | -1 |
| G: -6289.33611 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.45336 HOMO: -6.67767 LUMO: 1.70343 factor:1 | 1 (-0.75155) | -1 | -1 |
| G: -6289.33611 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.56604 HOMO: -6.37835 LUMO: 1.96466 factor:1 | 1 (-0.86423) | -1 | -1 |
| G: -6289.33611 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.59407 HOMO: -6.40828 LUMO: 2.10072 factor:1 | 1 (-0.89226) | -1 | -1 |
| G: -6289.33611 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.70833 HOMO: -6.06542 LUMO: 1.92112 factor:1 | 1 (-1.00652) | -1 | -1 |
| G: -6289.33611 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.32947 HOMO: -6.90353 LUMO: 1.83133 factor:1 | 1 (-0.62766) | -1 | -1 |
| G: -6289.33611 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.38666 HOMO: -6.37019 LUMO: 1.92929 factor:1 | 1 (-0.68486) | -1 | -1 |
| G: -6289.33611 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.43706 HOMO: -6.61509 LUMO: 2.11160 factor:1 | 1 (-0.73525) | -1 | -1 |
| G: -6289.33611 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.62566 HOMO: -6.82734 LUMO: 1.77146 factor:1 | 1 (-0.92385) | -1 | -1 |
| G: -6289.33611 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.51948 HOMO: -6.01100 LUMO: 1.89935 factor:1 | 1 (-0.81767) | -1 | -1 |
| G: -6289.33611 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.48922 HOMO: -6.49536 LUMO: 1.75241 factor:1 | 1 (-0.78742) | -1 | -1 |
| G: -6289.33611 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.33834 HOMO: -6.34297 LUMO: 1.86398 factor:1 | 1 (-0.63653) | -1 | -1 |
| G: -6289.33611 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.45330 HOMO: -6.53073 LUMO: 1.84493 factor:1 | 1 (-1.75149) | -1 | -1 |
| G: -6289.33611 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.46927 HOMO: -6.53345 LUMO: 2.41093 factor:1 | 1 (-1.76746) | -1 | -1 |
| G: -6289.33611 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.21560 HOMO: -7.01237 LUMO: 2.06262 factor:1 | 1 (-1.51380) | -1 | -1 |
| G: -6289.33611 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.54524 HOMO: -6.17154 LUMO: 1.89119 factor:1 | 1 (-1.84344) | -1 | -1 |
| G: -6289.33611 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.30859 HOMO: -6.08719 LUMO: 1.74425 factor:1 | 1 (-1.60678) | -1 | -1 |
| G: -6289.33611 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.15718 HOMO: -6.69672 LUMO: 1.95106 factor:1 | 1 (-1.45537) | -1 | -1 |
| G: -6289.33611 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.97383 HOMO: -6.58243 LUMO: 2.24766 factor:1 | 1 (-1.27202) | -1 | -1 |
| G: -6289.33611 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.38042 HOMO: -6.74570 LUMO: 2.02181 factor:1 | 1 (-1.67862) | -1 | -1 |
| G: -6289.33611 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.17073 HOMO: -6.53890 LUMO: 1.92929 factor:1 | 1 (-1.46893) | -1 | -1 |
| G: -6289.33611 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.34355 HOMO: -6.03276 LUMO: 1.67078 factor:1 | 1 (-1.64174) | -1 | -1 |
| G: -6289.33611 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.29865 HOMO: -6.67767 LUMO: 2.03541 factor:1 | 1 (-1.59685) | -1 | -1 |
| G: -6289.33611 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.10551 HOMO: -5.98378 LUMO: 1.84221 factor:1 | 1 (-1.40370) | -1 | -1 |
| G: -6289.33611 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.00766 HOMO: -6.07086 LUMO: 2.01908 factor:1 | 1 (-1.30585) | -1 | -1 |
| G: -6289.33611 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.39501 HOMO: -6.29944 LUMO: 1.90208 factor:1 | 1 (-1.69320) | -1 | -1 |
| G: -6289.33611 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.25174 HOMO: -6.75114 LUMO: 1.85854 factor:1 | 1 (-1.54993) | -1 | -1 |
| G: -6289.33611 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.95043 HOMO: -6.56611 LUMO: 2.49801 factor:1 | 1 (-1.24862) | -1 | -1 |
| G: -6289.33611 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.90599 HOMO: -6.39740 LUMO: 1.92929 factor:1 | 1 (-1.20419) | -1 | -1 |
| G: -6289.33611 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.79331 HOMO: -6.85999 LUMO: -1.07757 factor:1 | 1 (-1.09150) | -1 | -1 |
| G: -6289.33611 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.46476 HOMO: -6.98244 LUMO: 1.07213 factor:1 | 1 (-0.76295) | -1 | -1 |
| G: -6289.33611 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.19547 HOMO: -7.04231 LUMO: 0.64219 factor:1 | 1 (-1.49366) | -1 | -1 |
| G: -6289.33611 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.06020 HOMO: -6.96339 LUMO: 0.75648 factor:1 | 1 (-1.35839) | -1 | -1 |
| G: -6289.33611 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.85639 HOMO: -6.83822 LUMO: -0.97417 factor:1 | 1 (-1.15458) | -1 | -1 |
| G: -6289.33611 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.24048 HOMO: -6.44910 LUMO: -2.15242 factor:1 | 1 (-1.53867) | -1 | -1 |
| G: -6289.33611 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.06317 HOMO: -6.84094 LUMO: -1.37690 factor:1 | 1 (-1.36136) | -1 | -1 |
| G: -6289.33611 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.20154 HOMO: -6.74026 LUMO: -2.54699 factor:1 | 1 (-1.49973) | -1 | -1 |
| G: -6289.33611 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.41819 HOMO: -6.96611 LUMO: 1.24900 factor:1 | 1 (-1.71639) | -1 | -1 |
| G: -6289.33611 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.97078 HOMO: -7.21102 LUMO: 0.82995 factor:1 | 1 (-1.26898) | -1 | -1 |
| G: -6289.33611 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.90708 HOMO: -6.88448 LUMO: 0.81634 factor:1 | 1 (-1.20527) | -1 | -1 |
| G: -6289.33611 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.99133 HOMO: -7.04231 LUMO: 1.10750 factor:1 | 1 (-1.28952) | -1 | -1 |
| G: -6289.33611 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.35686 HOMO: -6.83550 LUMO: -0.98777 factor:1 | 1 (-1.65505) | -1 | -1 |
| G: -6289.33611 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.15615 HOMO: -6.82189 LUMO: 0.93879 factor:1 | 1 (-1.45434) | -1 | -1 |
| G: -6289.33611 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.22790 HOMO: -6.81101 LUMO: 0.70750 factor:1 | 1 (-1.52610) | -1 | -1 |
| G: -6289.33611 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.13960 HOMO: -7.06680 LUMO: 0.74015 factor:1 | 1 (-1.43780) | -1 | -1 |
| G: -6289.33611 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.36355 HOMO: -6.68856 LUMO: 0.86260 factor:1 | 1 (-1.66174) | -1 | -1 |
| G: -6289.33611 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.86058 HOMO: -6.83822 LUMO: -0.63403 factor:1 | 1 (-1.15877) | -1 | -1 |
| G: -6289.33611 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.73361 HOMO: -6.84911 LUMO: 1.26533 factor:1 | 1 (-1.03180) | -1 | -1 |
| G: -6289.33611 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.83489 HOMO: -7.01237 LUMO: 0.73743 factor:1 | 1 (-1.13308) | -1 | -1 |
| G: -6289.33611 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.46999 HOMO: -7.00965 LUMO: 1.40139 factor:1 | 1 (-0.76818) | -1 | -1 |
| G: -6289.33611 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.11628 HOMO: -6.73210 LUMO: -2.49256 factor:1 | 1 (-1.41448) | -1 | -1 |
| G: -6289.33611 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.91271 HOMO: -7.08040 LUMO: 0.84627 factor:1 | 1 (-1.21091) | -1 | -1 |
| G: -6289.33611 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.90833 HOMO: -7.00965 LUMO: 0.82995 factor:1 | 1 (-1.20653) | -1 | -1 |
| G: -6289.33611 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.82675 HOMO: -6.88448 LUMO: 0.82723 factor:1 | 1 (-1.12495) | -1 | -1 |
| G: -6289.33611 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.64019 HOMO: -7.20013 LUMO: 0.88437 factor:1 | 1 (-0.93838) | -1 | -1 |
| G: -6289.33611 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.11182 HOMO: -6.60420 LUMO: -0.53334 factor:1 | 1 (-1.41001) | -1 | -1 |
| G: -6289.33611 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.80557 HOMO: -6.78652 LUMO: -0.79729 factor:1 | 1 (-2.10377) | -1 | -1 |
| G: -6289.33611 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12556.58268 HOMO: -6.48992 LUMO: -0.64491 factor:1 | 1 (-2.88087) | -1 | -1 |
| G: -6289.33611 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.45983 HOMO: -6.85999 LUMO: -0.78097 factor:1 | 1 (-1.75802) | -1 | -1 |
| G: -6289.33611 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.60160 HOMO: -6.65046 LUMO: -0.78097 factor:1 | 1 (-1.89979) | -1 | -1 |
| G: -6289.33611 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.80664 HOMO: -7.24095 LUMO: 0.37280 factor:1 | 1 (-2.10483) | -1 | -1 |
| G: -6289.33611 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.39713 HOMO: -6.81101 LUMO: -0.74831 factor:1 | 1 (-1.69532) | -1 | -1 |
| G: -6289.33611 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.89643 HOMO: -6.69400 LUMO: -0.77280 factor:1 | 1 (-2.19463) | -1 | -1 |
| G: -6289.33611 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12556.40423 HOMO: -6.08447 LUMO: -0.68573 factor:1 | 1 (-2.70242) | -1 | -1 |
| G: -6289.33611 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12556.12193 HOMO: -6.66679 LUMO: -0.47076 factor:1 | 1 (-2.42013) | -1 | -1 |
| G: -6289.33611 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12556.58015 HOMO: -6.97428 LUMO: -1.10750 factor:1 | 1 (-2.87834) | -1 | -1 |
| G: -6289.33611 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.42173 HOMO: -6.69128 LUMO: -0.54151 factor:1 | 1 (-1.71992) | -1 | -1 |
| G: -6289.33611 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.23816 HOMO: -6.53617 LUMO: -0.35375 factor:1 | 1 (-1.53635) | -1 | -1 |
| G: -6289.33611 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.05566 HOMO: -6.75659 LUMO: -0.41361 factor:1 | 1 (-1.35385) | -1 | -1 |
| G: -6289.33611 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12556.52153 HOMO: -6.69400 LUMO: -0.67484 factor:1 | 1 (-2.81973) | -1 | -1 |
| G: -6289.33611 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.73961 HOMO: -6.89264 LUMO: -0.90886 factor:1 | 1 (-2.03781) | -1 | -1 |
| G: -6289.33611 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12556.66714 HOMO: -6.56339 LUMO: -0.52518 factor:1 | 1 (-2.96533) | -1 | -1 |
| G: -6289.33611 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.36274 HOMO: -6.45726 LUMO: -0.65852 factor:1 | 1 (-1.66093) | -1 | -1 |
| G: -6289.33611 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12556.13257 HOMO: -6.80557 LUMO: -0.56600 factor:1 | 1 (-2.43077) | -1 | -1 |
| G: -6289.33611 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.88773 HOMO: -7.19469 LUMO: -0.91702 factor:1 | 1 (-2.18592) | -1 | -1 |
| G: -6289.33611 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.67365 HOMO: -6.41100 LUMO: 0.79185 factor:1 | 1 (-1.97185) | -1 | -1 |
| G: -6289.33611 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.52623 HOMO: -6.39195 LUMO: 0.26123 factor:1 | 1 (-0.82442) | -1 | -1 |
| G: -6289.33611 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.39515 HOMO: -6.78924 LUMO: 0.35919 factor:1 | 1 (-0.69335) | -1 | -1 |
| G: -6289.33611 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.93986 HOMO: -6.50624 LUMO: 0.71838 factor:1 | 1 (-2.23805) | -1 | -1 |
| G: -6289.33611 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.39808 HOMO: -6.68584 LUMO: -0.66124 factor:1 | 1 (-1.69628) | -1 | -1 |
| G: -6289.33611 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.79034 HOMO: -6.45182 LUMO: -0.48980 factor:1 | 1 (-2.08853) | -1 | -1 |
| G: -6289.33611 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.34219 HOMO: -7.18925 LUMO: -1.01498 factor:1 | 1 (-1.64038) | -1 | -1 |
| G: -6289.33611 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.28611 HOMO: -7.18925 LUMO: -0.63130 factor:1 | 1 (-1.58430) | -1 | -1 |
| G: -6289.33611 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.39599 HOMO: -6.66679 LUMO: -0.57960 factor:1 | 1 (-1.69418) | -1 | -1 |
| G: -6289.33611 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.31789 HOMO: -6.44910 LUMO: -0.30205 factor:1 | 1 (-1.61608) | -1 | -1 |
| G: -6289.33611 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.45928 HOMO: -7.23279 LUMO: 0.46804 factor:1 | 1 (-1.75747) | -1 | -1 |
| G: -6289.33611 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.24505 HOMO: -6.92802 LUMO: -0.72927 factor:1 | 1 (-1.54324) | -1 | -1 |
| G: -6289.33611 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.11258 HOMO: -6.83278 LUMO: -0.59321 factor:1 | 1 (-1.41077) | -1 | -1 |
| G: -6289.33611 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.18151 HOMO: -7.44776 LUMO: 0.27211 factor:1 | 1 (-1.47970) | -1 | -1 |
| G: -6289.33611 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.89111 HOMO: -6.80829 LUMO: -0.59865 factor:1 | 1 (-1.18930) | -1 | -1 |
| G: -6289.33611 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.63368 HOMO: -6.63686 LUMO: -0.75103 factor:1 | 1 (-1.93187) | -1 | -1 |
| G: -6289.33611 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.82449 HOMO: -6.73210 LUMO: -0.55511 factor:1 | 1 (-2.12268) | -1 | -1 |
| G: -6289.33611 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.62680 HOMO: -6.50624 LUMO: 1.58642 factor:1 | 1 (-1.92499) | -1 | -1 |
| G: -6289.33611 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.85341 HOMO: -6.79196 LUMO: 0.96328 factor:1 | 1 (-2.15160) | -1 | -1 |
| G: -6289.33611 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12556.43340 HOMO: -6.82734 LUMO: 1.23540 factor:1 | 1 (-2.73159) | -1 | -1 |
| G: -6289.33611 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.65975 HOMO: -6.90081 LUMO: 1.25444 factor:1 | 1 (-1.95794) | -1 | -1 |
| G: -6289.33611 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12556.13021 HOMO: -7.00965 LUMO: -1.05036 factor:1 | 1 (-2.42840) | -1 | -1 |
| G: -6289.33611 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12556.21704 HOMO: -7.01237 LUMO: -1.48302 factor:1 | 1 (-2.51523) | -1 | -1 |
| G: -6289.33611 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.49700 HOMO: -6.91713 LUMO: 0.93607 factor:1 | 1 (-1.79519) | -1 | -1 |
| G: -6289.33611 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12556.06212 HOMO: -7.02598 LUMO: 0.92247 factor:1 | 1 (-2.36032) | -1 | -1 |
| G: -6289.33611 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.34369 HOMO: -6.98516 LUMO: 1.52384 factor:1 | 1 (-1.64188) | -1 | -1 |
| G: -6289.33611 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.41808 HOMO: -6.75387 LUMO: 1.04764 factor:1 | 1 (-1.71628) | -1 | -1 |
| G: -6289.33611 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.62152 HOMO: -7.09401 LUMO: 1.19458 factor:1 | 1 (-1.91971) | -1 | -1 |
| G: -6289.33611 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.46562 HOMO: -6.88992 LUMO: -1.56193 factor:1 | 1 (-1.76381) | -1 | -1 |
| G: -6289.33611 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.23713 HOMO: -7.00149 LUMO: 0.99866 factor:1 | 1 (-1.53532) | -1 | -1 |
| G: -6289.33611 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.25264 HOMO: -7.13755 LUMO: 1.05308 factor:1 | 1 (-1.55083) | -1 | -1 |
| G: -6289.33611 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.60455 HOMO: -6.85183 LUMO: -1.42860 factor:1 | 1 (-0.90274) | -1 | -1 |
| G: -6289.33611 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.38381 HOMO: -6.63141 LUMO: -0.88981 factor:1 | 1 (-0.68200) | -1 | -1 |
| G: -6289.33611 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.30209 HOMO: -6.92258 LUMO: -0.82178 factor:1 | 1 (-0.60028) | -1 | -1 |
| G: -6289.33611 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.56188 HOMO: -6.55794 LUMO: -0.80818 factor:1 | 1 (-0.86007) | -1 | -1 |
| G: -6289.33611 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.51208 HOMO: -6.95251 LUMO: -0.97145 factor:1 | 1 (-0.81027) | -1 | -1 |
| G: -6289.33611 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.11390 HOMO: -7.37701 LUMO: 0.14150 factor:1 | 1 (-0.41209) | -1 | -1 |
| G: -6289.33611 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.38879 HOMO: -6.74842 LUMO: -0.68028 factor:1 | 1 (-0.68698) | -1 | -1 |
| G: -6289.33611 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.31853 HOMO: -6.65046 LUMO: -0.52518 factor:1 | 1 (-0.61672) | -1 | -1 |
| G: -6289.33611 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.34990 HOMO: -6.91441 LUMO: -1.13199 factor:1 | 1 (-0.64809) | -1 | -1 |
| G: -6289.33611 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.18759 HOMO: -7.00965 LUMO: -1.00682 factor:1 | 1 (-0.48578) | -1 | -1 |
| G: -6289.33611 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.54659 HOMO: -6.55794 LUMO: -0.54967 factor:1 | 1 (-0.84478) | -1 | -1 |
| G: -6289.33611 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.32462 HOMO: -6.71577 LUMO: -0.53879 factor:1 | 1 (-0.62281) | -1 | -1 |
| G: -6289.33611 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.71787 HOMO: -6.88992 LUMO: -0.55511 factor:1 | 1 (-2.01606) | -1 | -1 |
| G: -6289.33611 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12556.50834 HOMO: -6.74026 LUMO: -0.60681 factor:1 | 1 (-2.80653) | -1 | -1 |
| G: -6289.33611 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12556.25900 HOMO: -6.76747 LUMO: -0.50885 factor:1 | 1 (-2.55719) | -1 | -1 |
| G: -6289.33611 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.60573 HOMO: -6.87904 LUMO: -0.92519 factor:1 | 1 (-1.90393) | -1 | -1 |
| G: -6289.33611 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.16707 HOMO: -6.53073 LUMO: -0.53062 factor:1 | 1 (-0.46526) | -1 | -1 |
| G: -6289.33611 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.39722 HOMO: -6.97700 LUMO: -0.98505 factor:1 | 1 (-0.69541) | -1 | -1 |
| G: -6289.33611 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.86778 HOMO: -6.96884 LUMO: -0.79185 factor:1 | 1 (-2.16597) | -1 | -1 |
| G: -6289.33611 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.19786 HOMO: -6.60420 LUMO: -0.31021 factor:1 | 1 (-1.49605) | -1 | -1 |
| G: -6289.33611 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12556.00384 HOMO: -6.68584 LUMO: -0.63947 factor:1 | 1 (-2.30203) | -1 | -1 |
| G: -6289.33611 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.90718 HOMO: -6.41917 LUMO: -0.35103 factor:1 | 1 (-2.20537) | -1 | -1 |
| G: -6289.33611 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.69028 HOMO: -6.73482 LUMO: -0.70477 factor:1 | 1 (-1.98847) | -1 | -1 |
| G: -6289.33611 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.97155 HOMO: -6.71305 LUMO: -0.85716 factor:1 | 1 (-1.26974) | -1 | -1 |
| G: -6289.33611 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.27920 HOMO: -6.70761 LUMO: -0.63403 factor:1 | 1 (-1.57739) | -1 | -1 |
| G: -6289.33611 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.40753 HOMO: -6.37563 LUMO: -0.38640 factor:1 | 1 (-1.70572) | -1 | -1 |
| G: -6289.33611 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.37204 HOMO: -6.27495 LUMO: -0.54967 factor:1 | 1 (-1.67023) | -1 | -1 |
| G: -6289.33611 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.35400 HOMO: -6.98516 LUMO: 0.38096 factor:1 | 1 (-1.65219) | -1 | -1 |
| G: -6289.33611 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.26965 HOMO: -6.47087 LUMO: -0.40001 factor:1 | 1 (-1.56784) | -1 | -1 |
| G: -6289.33611 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.56494 HOMO: -6.59876 LUMO: 0.20681 factor:1 | 1 (-1.86314) | -1 | -1 |
| G: -6289.33611 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.58816 HOMO: -6.89809 LUMO: 0.14966 factor:1 | 1 (-1.88635) | -1 | -1 |
| G: -6289.33611 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.36513 HOMO: -6.76203 LUMO: 2.11432 factor:1 | 1 (-1.66332) | -1 | -1 |
| G: -6289.33611 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.40862 HOMO: -6.58516 LUMO: 1.75786 factor:1 | 1 (-1.70681) | -1 | -1 |
| G: -6289.33611 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.10551 HOMO: -6.37835 LUMO: 1.84493 factor:1 | 1 (-1.40370) | -1 | -1 |
| G: -6289.33611 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.22761 HOMO: -6.83550 LUMO: 1.74425 factor:1 | 1 (-0.52581) | -1 | -1 |
| G: -6289.33611 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.08201 HOMO: -6.65318 LUMO: 1.79051 factor:1 | 1 (-0.38020) | -1 | -1 |
| G: -6289.33611 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.09991 HOMO: -6.68584 LUMO: 2.11160 factor:1 | 1 (-0.39810) | -1 | -1 |
| G: -6289.33611 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12553.83993 HOMO: -6.36202 LUMO: 1.85037 factor:1 | 1 (-0.13812) | -1 | -1 |
| G: -6289.33611 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.28459 HOMO: -6.68312 LUMO: 2.23133 factor:1 | 1 (-0.58279) | -1 | -1 |
| G: -6289.33611 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.99962 HOMO: -6.66679 LUMO: 2.14154 factor:1 | 1 (-2.29781) | -1 | -1 |
| G: -6289.33611 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.73978 HOMO: -6.50896 LUMO: 1.92657 factor:1 | 1 (-2.03797) | -1 | -1 |
| G: -6289.33611 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12556.05709 HOMO: -6.63686 LUMO: 2.22317 factor:1 | 1 (-2.35528) | -1 | -1 |
| G: -6289.33611 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.32848 HOMO: -6.58788 LUMO: 2.17419 factor:1 | 1 (-1.62667) | -1 | -1 |
| G: -6289.33611 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.05522 HOMO: -6.72665 LUMO: 2.12249 factor:1 | 1 (-1.35341) | -1 | -1 |
| G: -6289.33611 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.89976 HOMO: -6.28311 LUMO: 1.91024 factor:1 | 1 (-1.19795) | -1 | -1 |
| G: -6289.33611 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.09280 HOMO: -6.56067 LUMO: 2.27487 factor:1 | 1 (-1.39099) | -1 | -1 |
| G: -6289.33611 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.24516 HOMO: -6.83006 LUMO: 2.28031 factor:1 | 1 (-1.54335) | -1 | -1 |
| G: -6289.33611 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.22695 HOMO: -6.45182 LUMO: 1.62724 factor:1 | 1 (-1.52514) | -1 | -1 |
| G: -6289.33611 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.92885 HOMO: -6.78380 LUMO: 1.83677 factor:1 | 1 (-1.22704) | -1 | -1 |
| G: -6289.33611 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.04507 HOMO: -6.23413 LUMO: 1.80956 factor:1 | 1 (-1.34326) | -1 | -1 |
| G: -6289.33611 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.79405 HOMO: -6.74298 LUMO: 2.16875 factor:1 | 1 (-1.09224) | -1 | -1 |
| G: -6289.33611 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.23476 HOMO: -6.81645 LUMO: 2.50073 factor:1 | 1 (-1.53295) | -1 | -1 |
| G: -6289.33611 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.38944 HOMO: -6.71033 LUMO: 1.96466 factor:1 | 1 (-0.68763) | -1 | -1 |
| G: -6289.33611 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.58509 HOMO: -6.83550 LUMO: 2.04358 factor:1 | 1 (-0.88328) | -1 | -1 |
| G: -6289.33611 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.52014 HOMO: -6.60965 LUMO: 2.38100 factor:1 | 1 (-0.81833) | -1 | -1 |
| G: -6289.33611 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.48637 HOMO: -6.73210 LUMO: 2.26127 factor:1 | 1 (-0.78456) | -1 | -1 |
| G: -6289.33611 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.19240 HOMO: -6.76203 LUMO: 2.13609 factor:1 | 1 (-0.49059) | -1 | -1 |
| G: -6289.33611 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.33186 HOMO: -6.71033 LUMO: 2.05990 factor:1 | 1 (-0.63005) | -1 | -1 |
| G: -6289.33611 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.55497 HOMO: -6.50896 LUMO: 2.32385 factor:1 | 1 (-0.85316) | -1 | -1 |
| G: -6289.33611 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.78414 HOMO: -6.53345 LUMO: 1.74425 factor:1 | 1 (-1.08233) | -1 | -1 |
| G: -6289.33611 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.75535 HOMO: -6.25862 LUMO: 1.63540 factor:1 | 1 (-1.05354) | -1 | -1 |
| G: -6289.33611 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.48022 HOMO: -5.90759 LUMO: 1.78779 factor:1 | 1 (-0.77841) | -1 | -1 |
| G: -6289.33611 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.55739 HOMO: -6.09807 LUMO: 1.99732 factor:1 | 1 (-0.85558) | -1 | -1 |
| G: -6289.33611 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.23123 HOMO: -5.92392 LUMO: 1.99732 factor:1 | 1 (-0.52942) | -1 | -1 |
| G: -6289.33611 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.33513 HOMO: -6.45182 LUMO: 1.72248 factor:1 | 1 (-0.63332) | -1 | -1 |
| G: -6289.33611 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.20522 HOMO: -6.53073 LUMO: 1.82588 factor:1 | 1 (-0.50341) | -1 | -1 |
| G: -6289.33611 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.04503 HOMO: -6.40828 LUMO: 2.05174 factor:1 | 1 (-0.34322) | -1 | -1 |
| G: -6289.33611 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.33567 HOMO: -6.60420 LUMO: -0.82450 factor:1 | 1 (-0.63386) | -1 | -1 |
| G: -6289.33611 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.57415 HOMO: -6.76747 LUMO: -0.57144 factor:1 | 1 (-0.87234) | -1 | -1 |
| G: -6289.33611 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.62776 HOMO: -6.67767 LUMO: -0.59321 factor:1 | 1 (-0.92595) | -1 | -1 |
| G: -6289.33611 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.35330 HOMO: -6.65863 LUMO: -0.57416 factor:1 | 1 (-0.65150) | -1 | -1 |
| G: -6289.33611 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.57284 HOMO: -6.49808 LUMO: -0.54695 factor:1 | 1 (-0.87104) | -1 | -1 |
| G: -6289.33611 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.47042 HOMO: -6.50080 LUMO: -0.61498 factor:1 | 1 (-0.76861) | -1 | -1 |
| G: -6289.33611 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.67026 HOMO: -6.74842 LUMO: -0.51974 factor:1 | 1 (-0.96845) | -1 | -1 |
| G: -6289.33611 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.17052 HOMO: -6.13345 LUMO: 0.67756 factor:1 | 1 (-1.46871) | -1 | -1 |
| G: -6289.33611 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.33591 HOMO: -6.48719 LUMO: 0.52790 factor:1 | 1 (-1.63410) | -1 | -1 |
| G: -6289.33611 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.04330 HOMO: -6.35930 LUMO: 0.74015 factor:1 | 1 (-1.34149) | -1 | -1 |
| G: -6289.33611 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.11054 HOMO: -6.41644 LUMO: 0.22313 factor:1 | 1 (-1.40873) | -1 | -1 |
| G: -6289.33611 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.02442 HOMO: -6.85727 LUMO: -0.00272 factor:1 | 1 (-1.32261) | -1 | -1 |
| G: -6289.33611 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.08181 HOMO: -6.84638 LUMO: 0.24762 factor:1 | 1 (-1.38000) | -1 | -1 |
| G: -6289.33611 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.56985 HOMO: -6.66951 LUMO: 0.39184 factor:1 | 1 (-0.86804) | -1 | -1 |
| G: -6289.33611 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.31379 HOMO: -6.62597 LUMO: -0.65035 factor:1 | 1 (-0.61198) | -1 | -1 |
| G: -6289.33611 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.13295 HOMO: -7.13755 LUMO: 0.45715 factor:1 | 1 (-0.43114) | -1 | -1 |
| G: -6289.33611 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12553.95498 HOMO: -7.12666 LUMO: 0.45171 factor:1 | 1 (-0.25317) | -1 | -1 |
| G: -6289.33611 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.25401 HOMO: -6.46270 LUMO: -0.46259 factor:1 | 1 (-0.55220) | -1 | -1 |
| G: -6289.33611 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.38432 HOMO: -6.36202 LUMO: -0.29660 factor:1 | 1 (-0.68252) | -1 | -1 |
| G: -6289.33611 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.34198 HOMO: -6.28583 LUMO: 0.40545 factor:1 | 1 (-0.64018) | -1 | -1 |
| G: -6289.33611 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.29774 HOMO: -6.70761 LUMO: 0.41906 factor:1 | 1 (-0.59593) | -1 | -1 |
| G: -6289.33611 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.05771 HOMO: -6.76203 LUMO: -0.60954 factor:1 | 1 (-0.35590) | -1 | -1 |
| G: -6289.33611 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.25414 HOMO: -6.85999 LUMO: -0.75103 factor:1 | 1 (-0.55234) | -1 | -1 |
| G: -6289.33611 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.15757 HOMO: -7.19741 LUMO: -1.00954 factor:1 | 1 (-0.45576) | -1 | -1 |
| G: -6289.33611 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12553.84864 HOMO: -6.58243 LUMO: -0.33470 factor:1 | 1 (-0.14683) | -1 | -1 |
| G: -6289.33611 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.50375 HOMO: -7.22190 LUMO: 0.49253 factor:1 | 1 (-0.80195) | -1 | -1 |
| G: -6289.33611 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.16968 HOMO: -7.22462 LUMO: 0.51974 factor:1 | 1 (-0.46787) | -1 | -1 |
| G: -6289.33611 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.49959 HOMO: -7.08584 LUMO: -0.68301 factor:1 | 1 (-0.79778) | -1 | -1 |
| G: -6289.33611 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.33608 HOMO: -6.68584 LUMO: -0.29660 factor:1 | 1 (-0.63427) | -1 | -1 |
| G: -6289.33611 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.13009 HOMO: -6.33753 LUMO: -0.48436 factor:1 | 1 (-0.42828) | -1 | -1 |
| G: -6289.33611 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12553.82959 HOMO: -7.15932 LUMO: 0.55511 factor:1 | 1 (-0.12778) | -1 | -1 |
| G: -6289.33611 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.32528 HOMO: -6.57427 LUMO: 2.01908 factor:1 | 1 (-0.62347) | -1 | -1 |
| G: -6289.33611 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.51233 HOMO: -6.75659 LUMO: 2.22045 factor:1 | 1 (-0.81052) | -1 | -1 |
| G: -6289.33611 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.45235 HOMO: -6.73482 LUMO: 2.20956 factor:1 | 1 (-0.75054) | -1 | -1 |
| G: -6289.33611 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.26253 HOMO: -6.74026 LUMO: 1.76602 factor:1 | 1 (-0.56072) | -1 | -1 |
| G: -6289.33611 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.26508 HOMO: -6.95523 LUMO: 1.94834 factor:1 | 1 (-0.56328) | -1 | -1 |
| G: -6289.33611 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12553.90959 HOMO: -6.33209 LUMO: 1.87486 factor:1 | 1 (-0.20779) | -1 | -1 |
| G: -6289.33611 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.08103 HOMO: -6.71033 LUMO: 2.12521 factor:1 | 1 (-0.37922) | -1 | -1 |
| G: -6289.33611 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.10432 HOMO: -6.50080 LUMO: 2.04902 factor:1 | 1 (-0.40251) | -1 | -1 |
| G: -6289.33611 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12553.83237 HOMO: -6.76475 LUMO: 1.94017 factor:1 | 1 (-0.13056) | -1 | -1 |
| G: -6289.33611 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.36974 HOMO: -6.53073 LUMO: 2.08983 factor:1 | 1 (-0.66793) | -1 | -1 |
| G: -6289.33611 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.66830 HOMO: -6.69944 LUMO: 2.20684 factor:1 | 1 (-0.96649) | -1 | -1 |
| G: -6289.33611 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.43494 HOMO: -6.34570 LUMO: 1.80684 factor:1 | 1 (-0.73313) | -1 | -1 |
| G: -6289.33611 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.58071 HOMO: -6.78380 LUMO: 1.95922 factor:1 | 1 (-0.87890) | -1 | -1 |
| G: -6289.33611 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.66626 HOMO: -6.93618 LUMO: 1.76058 factor:1 | 1 (-0.96445) | -1 | -1 |
| G: -6289.33611 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.72863 HOMO: -6.93346 LUMO: 1.79595 factor:1 | 1 (-1.02682) | -1 | -1 |
| G: -6289.33611 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.43926 HOMO: -6.29671 LUMO: 1.75241 factor:1 | 1 (-0.73746) | -1 | -1 |
| G: -6289.33611 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.39200 HOMO: -6.77019 LUMO: 1.74697 factor:1 | 1 (-0.69019) | -1 | -1 |
| G: -6289.33611 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.64134 HOMO: -6.87360 LUMO: 1.91024 factor:1 | 1 (-0.93953) | -1 | -1 |
| G: -6289.33611 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.34030 HOMO: -6.32665 LUMO: 1.87759 factor:1 | 1 (-0.63849) | -1 | -1 |
| G: -6289.33611 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.58479 HOMO: -6.99877 LUMO: 1.99187 factor:1 | 1 (-0.88298) | -1 | -1 |
| G: -6289.33611 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.62939 HOMO: -6.72665 LUMO: 2.12521 factor:1 | 1 (-0.92758) | -1 | -1 |
| G: -6289.33611 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.41983 HOMO: -6.67767 LUMO: 2.43814 factor:1 | 1 (-0.71803) | -1 | -1 |
| G: -6289.33611 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.28323 HOMO: -6.99605 LUMO: 1.79051 factor:1 | 1 (-0.58143) | -1 | -1 |
| G: -6289.33611 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.36514 HOMO: -6.25046 LUMO: 1.77146 factor:1 | 1 (-0.66333) | -1 | -1 |
| G: -6289.33611 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.48258 HOMO: -6.30488 LUMO: 1.90480 factor:1 | 1 (-0.78078) | -1 | -1 |
| G: -6289.33611 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.52792 HOMO: -6.38379 LUMO: 1.68438 factor:1 | 1 (-0.82611) | -1 | -1 |
| G: -6289.33611 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.32729 HOMO: -6.78924 LUMO: 2.01364 factor:1 | 1 (-0.62548) | -1 | -1 |
| G: -6289.33611 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.14002 HOMO: -6.15249 LUMO: 1.98643 factor:1 | 1 (-0.43821) | -1 | -1 |
| G: -6289.33611 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12553.86426 HOMO: -6.19331 LUMO: 2.14154 factor:1 | 1 (-0.16245) | -1 | -1 |
| G: -6289.33611 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.39219 HOMO: -6.05998 LUMO: 2.12521 factor:1 | 1 (-0.69038) | -1 | -1 |
| G: -6289.33611 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.37025 HOMO: -6.67223 LUMO: 1.91840 factor:1 | 1 (-1.66844) | -1 | -1 |
| G: -6289.33611 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.39411 HOMO: -6.79196 LUMO: 2.18507 factor:1 | 1 (-1.69230) | -1 | -1 |
| G: -6289.33611 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.37863 HOMO: -6.93346 LUMO: 1.78235 factor:1 | 1 (-1.67682) | -1 | -1 |
| G: -6289.33611 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.95620 HOMO: -6.16882 LUMO: 1.80956 factor:1 | 1 (-1.25439) | -1 | -1 |
| G: -6289.33611 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.18173 HOMO: -6.72665 LUMO: 2.07895 factor:1 | 1 (-1.47992) | -1 | -1 |
| G: -6289.33611 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.09231 HOMO: -6.73210 LUMO: 1.97827 factor:1 | 1 (-1.39050) | -1 | -1 |
| G: -6289.33611 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.16377 HOMO: -6.84638 LUMO: 1.87214 factor:1 | 1 (-1.46196) | -1 | -1 |
| G: -6289.33611 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.60196 HOMO: -6.83006 LUMO: 2.36195 factor:1 | 1 (-0.90015) | -1 | -1 |
| G: -6289.33611 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.35189 HOMO: -6.97700 LUMO: 1.91024 factor:1 | 1 (-0.65008) | -1 | -1 |
| G: -6289.33611 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.38612 HOMO: -6.20420 LUMO: 1.81772 factor:1 | 1 (-0.68431) | -1 | -1 |
| G: -6289.33611 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.20595 HOMO: -7.09129 LUMO: 2.10344 factor:1 | 1 (-0.50415) | 1 | 1 |
| G: -6289.33611 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.16097 HOMO: -6.77564 LUMO: 2.14970 factor:1 | 1 (-0.45916) | -1 | -1 |
| G: -6289.33611 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.10116 HOMO: -6.81645 LUMO: 1.85854 factor:1 | 1 (-0.39935) | -1 | -1 |
| G: -6289.33611 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12553.93531 HOMO: -6.50896 LUMO: 2.04358 factor:1 | 1 (-0.23350) | -1 | -1 |
| G: -6289.33611 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.35110 HOMO: -6.89264 LUMO: 1.66262 factor:1 | 1 (-0.64929) | -1 | -1 |
| G: -6289.33611 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.32440 HOMO: -6.75931 LUMO: 2.23950 factor:1 | 1 (-0.62260) | -1 | -1 |
| G: -6289.33611 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.20744 HOMO: -6.50080 LUMO: 1.67622 factor:1 | 1 (-1.50563) | -1 | -1 |
| G: -6289.33611 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.05487 HOMO: -6.30216 LUMO: 2.24222 factor:1 | 1 (-1.35306) | -1 | -1 |
| G: -6289.33611 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.49463 HOMO: -7.18108 LUMO: 2.10072 factor:1 | 1 (-1.79282) | 1 | 1 |
| G: -6289.33611 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.84360 HOMO: -6.54162 LUMO: 2.35378 factor:1 | 1 (-1.14179) | -1 | -1 |
| G: -6289.33611 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.88308 HOMO: -5.98650 LUMO: 1.48302 factor:1 | 1 (-1.18127) | -1 | -1 |
| G: -6289.33611 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.97971 HOMO: -7.15115 LUMO: 2.14970 factor:1 | 1 (-1.27790) | 1 | 1 |
| G: -6289.33611 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.00752 HOMO: -6.45454 LUMO: 2.15786 factor:1 | 1 (-1.30571) | -1 | -1 |
| G: -6289.33611 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.14012 HOMO: -7.06952 LUMO: 2.14970 factor:1 | 1 (-1.43831) | 1 | 1 |
| G: -6289.33611 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.13383 HOMO: -6.93618 LUMO: 1.86942 factor:1 | 1 (-1.43203) | -1 | -1 |
| G: -6289.33611 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.04123 HOMO: -6.63141 LUMO: 1.92657 factor:1 | 1 (-1.33943) | -1 | -1 |
| G: -6289.33611 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.98518 HOMO: -6.51441 LUMO: -0.44355 factor:1 | 1 (-1.28337) | -1 | -1 |
| G: -6289.33611 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.75995 HOMO: -6.82734 LUMO: -1.03131 factor:1 | 1 (-1.05814) | -1 | -1 |
| G: -6289.33611 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.87633 HOMO: -6.58788 LUMO: -0.82995 factor:1 | 1 (-1.17453) | -1 | -1 |
| G: -6289.33611 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.93152 HOMO: -6.43277 LUMO: -0.40817 factor:1 | 1 (-1.22971) | -1 | -1 |
| G: -6289.33611 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.22355 HOMO: -6.78924 LUMO: -0.72110 factor:1 | 1 (-1.52174) | -1 | -1 |
| G: -6289.33611 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.00306 HOMO: -7.28177 LUMO: 0.36735 factor:1 | 1 (-1.30125) | -1 | -1 |
| G: -6289.33611 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.05166 HOMO: -6.47903 LUMO: -0.46259 factor:1 | 1 (-1.34985) | -1 | -1 |
| G: -6289.33611 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.29898 HOMO: -6.67495 LUMO: -0.75376 factor:1 | 1 (-1.59717) | -1 | -1 |
| G: -6289.33611 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12556.42110 HOMO: -6.71033 LUMO: -0.71838 factor:1 | 1 (-2.71929) | -1 | -1 |
| G: -6289.33611 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.79624 HOMO: -6.79740 LUMO: -0.79185 factor:1 | 1 (-2.09443) | -1 | -1 |
| G: -6289.33611 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12556.57737 HOMO: -6.08719 LUMO: -0.63675 factor:1 | 1 (-2.87556) | -1 | -1 |
| G: -6289.33611 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.59235 HOMO: -6.84094 LUMO: 0.42994 factor:1 | 1 (-1.89054) | -1 | -1 |
| G: -6289.33611 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.61006 HOMO: -6.59604 LUMO: 0.25851 factor:1 | 1 (-1.90825) | -1 | -1 |
| G: -6289.33611 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12556.43644 HOMO: -6.82462 LUMO: 0.08708 factor:1 | 1 (-2.73464) | -1 | -1 |
| G: -6289.33611 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12556.39827 HOMO: -6.54706 LUMO: 0.44082 factor:1 | 1 (-2.69646) | -1 | -1 |
| G: -6289.33611 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12556.01633 HOMO: -6.99333 LUMO: 0.32109 factor:1 | 1 (-2.31452) | -1 | -1 |
| G: -6289.33611 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12556.39759 HOMO: -6.29944 LUMO: -0.57144 factor:1 | 1 (-2.69578) | -1 | -1 |
| G: -6289.33611 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12556.20077 HOMO: -6.57699 LUMO: -0.46531 factor:1 | 1 (-2.49896) | -1 | -1 |
| G: -6289.33611 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.41242 HOMO: -6.24773 LUMO: -0.53879 factor:1 | 1 (-1.71062) | -1 | -1 |
| G: -6289.33611 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.98346 HOMO: -6.96067 LUMO: -0.67212 factor:1 | 1 (-1.28166) | -1 | -1 |
| G: -6289.33611 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12556.16076 HOMO: -7.24095 LUMO: -0.09252 factor:1 | 1 (-2.45896) | -1 | -1 |
| G: -6289.33611 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.26867 HOMO: -6.33481 LUMO: -0.46531 factor:1 | 1 (-1.56686) | -1 | -1 |
| G: -6289.33611 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.42004 HOMO: -6.43549 LUMO: -0.33198 factor:1 | 1 (-1.71824) | -1 | -1 |
| G: -6289.33611 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.04847 HOMO: -6.53073 LUMO: 0.44899 factor:1 | 1 (-1.34666) | -1 | -1 |
| G: -6289.33611 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.61213 HOMO: -6.69128 LUMO: 0.47620 factor:1 | 1 (-1.91032) | -1 | -1 |
| G: -6289.33611 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.33278 HOMO: -6.65318 LUMO: 0.52246 factor:1 | 1 (-1.63097) | -1 | -1 |
| G: -6289.33611 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.43545 HOMO: -6.71305 LUMO: 0.41089 factor:1 | 1 (-1.73364) | -1 | -1 |
| G: -6289.33611 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.48143 HOMO: -6.70216 LUMO: 0.19864 factor:1 | 1 (-1.77962) | -1 | -1 |
| G: -6289.33611 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.35574 HOMO: -6.41100 LUMO: 0.34558 factor:1 | 1 (-1.65394) | -1 | -1 |
| G: -6289.33611 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.79926 HOMO: -7.01237 LUMO: 0.02993 factor:1 | 1 (-2.09745) | -1 | -1 |
| G: -6289.33611 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.60688 HOMO: -6.85999 LUMO: 0.18776 factor:1 | 1 (-1.90507) | -1 | -1 |
| G: -6289.33611 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.64473 HOMO: -6.62869 LUMO: 0.48708 factor:1 | 1 (-1.94292) | -1 | -1 |
| G: -6289.33611 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.61575 HOMO: -6.43821 LUMO: -0.45715 factor:1 | 1 (-1.91394) | -1 | -1 |
| G: -6289.33611 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.23956 HOMO: -6.43277 LUMO: -0.72110 factor:1 | 1 (-0.53775) | -1 | -1 |
| G: -6289.33611 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.40013 HOMO: -7.10761 LUMO: 0.43266 factor:1 | 1 (-0.69833) | -1 | -1 |
| G: -6289.33611 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.24974 HOMO: -6.57699 LUMO: -0.61498 factor:1 | 1 (-0.54793) | -1 | -1 |
| G: -6289.33611 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.44525 HOMO: -6.82189 LUMO: -0.75648 factor:1 | 1 (-0.74344) | -1 | -1 |
| G: -6289.33611 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.32143 HOMO: -6.55794 LUMO: -0.67212 factor:1 | 1 (-1.61962) | -1 | -1 |
| G: -6289.33611 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12556.03823 HOMO: -6.69128 LUMO: 1.88575 factor:1 | 1 (-2.33642) | -1 | -1 |
| G: -6289.33611 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.97173 HOMO: -6.65591 LUMO: 1.70888 factor:1 | 1 (-2.26992) | -1 | -1 |
| G: -6289.33611 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.33612 HOMO: -6.58788 LUMO: 1.68438 factor:1 | 1 (-1.63432) | -1 | -1 |
| G: -6289.33611 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.81398 HOMO: -6.46270 LUMO: 1.72520 factor:1 | 1 (-2.11217) | -1 | -1 |
| G: -6289.33611 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.16886 HOMO: -6.57427 LUMO: 1.73881 factor:1 | 1 (-1.46705) | -1 | -1 |
| G: -6289.33611 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.36393 HOMO: -6.45182 LUMO: 1.75241 factor:1 | 1 (-1.66213) | -1 | -1 |
| G: -6289.33611 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.28576 HOMO: -6.51441 LUMO: 1.78779 factor:1 | 1 (-1.58395) | -1 | -1 |
| G: -6289.33611 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.25599 HOMO: -6.67495 LUMO: 2.11705 factor:1 | 1 (-1.55418) | -1 | -1 |
| G: -6289.33611 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.29974 HOMO: -6.22597 LUMO: 1.96466 factor:1 | 1 (-1.59793) | -1 | -1 |
| G: -6289.33611 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.93582 HOMO: -6.68040 LUMO: 2.30753 factor:1 | 1 (-1.23401) | -1 | -1 |
| G: -6289.33611 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.07421 HOMO: -6.65046 LUMO: 2.18235 factor:1 | 1 (-1.37241) | -1 | -1 |
| G: -6289.33611 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.04017 HOMO: -6.38651 LUMO: 1.76874 factor:1 | 1 (-1.33836) | -1 | -1 |
| G: -6289.33611 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.86632 HOMO: -6.41644 LUMO: 2.09256 factor:1 | 1 (-1.16451) | -1 | -1 |
| G: -6289.33611 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.26083 HOMO: -6.14977 LUMO: 2.28031 factor:1 | 1 (-1.55902) | -1 | -1 |
| G: -6289.33611 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.38555 HOMO: -6.70489 LUMO: 2.43814 factor:1 | 1 (-0.68374) | -1 | -1 |
| G: -6289.33611 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.45328 HOMO: -6.78924 LUMO: 2.27215 factor:1 | 1 (-0.75147) | -1 | -1 |
| G: -6289.33611 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.25058 HOMO: -6.86271 LUMO: 2.31025 factor:1 | 1 (-0.54877) | -1 | -1 |
| G: -6289.33611 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.45698 HOMO: -6.51168 LUMO: 2.04630 factor:1 | 1 (-0.75517) | -1 | -1 |
| G: -6289.33611 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.30566 HOMO: -6.72665 LUMO: 2.13337 factor:1 | 1 (-0.60385) | -1 | -1 |
| G: -6289.33611 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.44824 HOMO: -6.45998 LUMO: 2.16058 factor:1 | 1 (-0.74644) | -1 | -1 |
| G: -6289.33611 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.22242 HOMO: -6.83822 LUMO: 2.20684 factor:1 | 1 (-0.52061) | -1 | -1 |
| G: -6289.33611 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.42819 HOMO: -6.68856 LUMO: 2.19324 factor:1 | 1 (-0.72638) | -1 | -1 |
| G: -6289.33611 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.32177 HOMO: -6.71577 LUMO: 2.16058 factor:1 | 1 (-0.61996) | -1 | -1 |
| G: -6289.33611 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.26503 HOMO: -6.82462 LUMO: 1.90208 factor:1 | 1 (-0.56322) | -1 | -1 |
| G: -6289.33611 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.46318 HOMO: -6.61509 LUMO: 2.23950 factor:1 | 1 (-0.76137) | -1 | -1 |
| G: -6289.33611 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.29115 HOMO: -6.73754 LUMO: 1.84221 factor:1 | 1 (-0.58934) | -1 | -1 |
| G: -6289.33611 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.26315 HOMO: -6.56611 LUMO: 1.94561 factor:1 | 1 (-0.56134) | -1 | -1 |
| G: -6289.33611 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.31172 HOMO: -6.67767 LUMO: 1.51840 factor:1 | 1 (-0.60992) | -1 | -1 |
| G: -6289.33611 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.23423 HOMO: -6.35658 LUMO: 2.16603 factor:1 | 1 (-0.53242) | -1 | -1 |
| G: -6289.33611 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.36865 HOMO: -6.35114 LUMO: 2.08983 factor:1 | 1 (-0.66684) | -1 | -1 |
| G: -6289.33611 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.31276 HOMO: -6.35114 LUMO: 2.10616 factor:1 | 1 (-0.61095) | -1 | -1 |
| G: -6289.33611 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.51565 HOMO: -6.71305 LUMO: 2.01636 factor:1 | 1 (-0.81384) | -1 | -1 |
| G: -6289.33611 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.41026 HOMO: -6.24773 LUMO: 1.98915 factor:1 | 1 (-0.70845) | -1 | -1 |
| G: -6289.33611 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.28922 HOMO: -6.53617 LUMO: 2.42726 factor:1 | 1 (-0.58741) | -1 | -1 |
| G: -6289.33611 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12553.97528 HOMO: -6.59332 LUMO: 1.82316 factor:1 | 1 (-0.27347) | -1 | -1 |
| G: -6289.33611 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.20859 HOMO: -6.41372 LUMO: 1.77418 factor:1 | 1 (-0.50678) | -1 | -1 |
| G: -6289.33611 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.40326 HOMO: -6.40284 LUMO: 1.88575 factor:1 | 1 (-0.70146) | -1 | -1 |
| G: -6289.33611 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.19643 HOMO: -6.11168 LUMO: 1.70888 factor:1 | 1 (-0.49462) | -1 | -1 |
| G: -6289.33611 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.41047 HOMO: -6.44910 LUMO: 2.23405 factor:1 | 1 (-0.70867) | -1 | -1 |
| G: -6289.33611 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.32620 HOMO: -6.24773 LUMO: 2.12793 factor:1 | 1 (-0.62439) | -1 | -1 |
| G: -6289.33611 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.23409 HOMO: -6.07358 LUMO: 1.89663 factor:1 | 1 (-0.53228) | -1 | -1 |
| G: -6289.33611 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.43760 HOMO: -6.66679 LUMO: 1.96738 factor:1 | 1 (-0.73580) | -1 | -1 |
| G: -6289.33611 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.50642 HOMO: -6.68312 LUMO: 1.78235 factor:1 | 1 (-0.80461) | -1 | -1 |
| G: -6289.33611 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.96665 HOMO: -6.70761 LUMO: 1.97555 factor:1 | 1 (-1.26484) | -1 | -1 |
| G: -6289.33611 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.04978 HOMO: -6.15794 LUMO: 2.00548 factor:1 | 1 (-1.34797) | -1 | -1 |
| G: -6289.33611 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.90112 HOMO: -6.52257 LUMO: 1.96738 factor:1 | 1 (-1.19931) | -1 | -1 |
| G: -6289.33611 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.00159 HOMO: -6.25590 LUMO: 1.86670 factor:1 | 1 (-1.29978) | -1 | -1 |
| G: -6289.33611 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.08730 HOMO: -6.30216 LUMO: 1.84765 factor:1 | 1 (-1.38549) | -1 | -1 |
| G: -6289.33611 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.22344 HOMO: -6.76747 LUMO: 2.20956 factor:1 | 1 (-1.52163) | -1 | -1 |
| G: -6289.33611 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.36336 HOMO: -6.14161 LUMO: 1.80684 factor:1 | 1 (-1.66155) | -1 | -1 |
| G: -6289.33611 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.96719 HOMO: -6.81373 LUMO: 1.91024 factor:1 | 1 (-1.26538) | -1 | -1 |
| G: -6289.33611 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.45822 HOMO: -6.81917 LUMO: 2.34834 factor:1 | 1 (-1.75641) | -1 | -1 |
| G: -6289.33611 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12556.38678 HOMO: -6.72121 LUMO: 1.90208 factor:1 | 1 (-2.68497) | -1 | -1 |
| G: -6289.33611 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12556.16795 HOMO: -7.51851 LUMO: 0.26939 factor:1 | 1 (-2.46614) | -1 | -1 |
| G: -6289.33611 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12556.42335 HOMO: -6.65318 LUMO: -0.57144 factor:1 | 1 (-2.72155) | -1 | -1 |
| G: -6289.33611 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.50184 HOMO: -6.77564 LUMO: -0.72654 factor:1 | 1 (-1.80003) | -1 | -1 |
| G: -6289.33611 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12556.01902 HOMO: -6.80557 LUMO: -0.60954 factor:1 | 1 (-2.31721) | -1 | -1 |
| G: -6289.33611 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.41030 HOMO: -7.35524 LUMO: 0.27483 factor:1 | 1 (-1.70849) | -1 | -1 |
| G: -6289.33611 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12556.20528 HOMO: -6.94979 LUMO: -0.83811 factor:1 | 1 (-2.50347) | -1 | -1 |
| G: -6289.33611 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12556.26485 HOMO: -6.13345 LUMO: -0.67212 factor:1 | 1 (-2.56304) | -1 | -1 |
| G: -6289.33611 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.24129 HOMO: -6.47359 LUMO: -0.59321 factor:1 | 1 (-1.53948) | -1 | -1 |
| G: -6289.33611 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12556.05448 HOMO: -6.52257 LUMO: -0.54695 factor:1 | 1 (-2.35267) | -1 | -1 |
| G: -6289.33611 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.45700 HOMO: -6.61781 LUMO: -0.69661 factor:1 | 1 (-1.75519) | -1 | -1 |
| G: -6289.33611 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.27988 HOMO: -6.77564 LUMO: -0.80001 factor:1 | 1 (-1.57807) | -1 | -1 |
| G: -6289.33611 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.18823 HOMO: -7.35252 LUMO: -1.00410 factor:1 | 1 (-1.48642) | -1 | -1 |
| G: -6289.33611 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.34099 HOMO: -6.35386 LUMO: -0.38912 factor:1 | 1 (-1.63919) | -1 | -1 |
| G: -6289.33611 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.40932 HOMO: -6.80285 LUMO: -0.52246 factor:1 | 1 (-1.70751) | -1 | -1 |
| G: -6289.33611 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.26045 HOMO: -7.23279 LUMO: 0.30477 factor:1 | 1 (-1.55864) | -1 | -1 |
| G: -6289.33611 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.96940 HOMO: -7.13483 LUMO: -0.76192 factor:1 | 1 (-1.26759) | -1 | -1 |
| G: -6289.33611 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.46758 HOMO: -6.71849 LUMO: -0.48164 factor:1 | 1 (-1.76577) | -1 | -1 |
| G: -6289.33611 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.38114 HOMO: -6.85455 LUMO: -0.69389 factor:1 | 1 (-0.67933) | -1 | -1 |
| G: -6289.33611 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.39728 HOMO: -6.96339 LUMO: -0.73743 factor:1 | 1 (-0.69547) | -1 | -1 |
| G: -6289.33611 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.35328 HOMO: -7.50490 LUMO: 0.28844 factor:1 | 1 (-0.65147) | -1 | -1 |
| G: -6289.33611 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12553.98236 HOMO: -6.63958 LUMO: -0.50069 factor:1 | 1 (-0.28055) | -1 | -1 |
| G: -6289.33611 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.16582 HOMO: -6.78924 LUMO: -0.69661 factor:1 | 1 (-0.46401) | -1 | -1 |
| G: -6289.33611 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.25055 HOMO: -7.44776 LUMO: 0.33742 factor:1 | 1 (-0.54874) | -1 | -1 |
| G: -6289.33611 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12553.91675 HOMO: -6.15249 LUMO: 0.66396 factor:1 | 1 (-0.21494) | -1 | -1 |
| G: -6289.33611 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.11776 HOMO: -6.17426 LUMO: 0.55511 factor:1 | 1 (-0.41595) | -1 | -1 |
| G: -6289.33611 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.27458 HOMO: -6.83550 LUMO: 0.28844 factor:1 | 1 (-0.57277) | -1 | -1 |
| G: -6289.33611 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.17681 HOMO: -6.32393 LUMO: 0.47620 factor:1 | 1 (-0.47500) | -1 | -1 |
| G: -6289.33611 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.62326 HOMO: -6.32937 LUMO: 0.45987 factor:1 | 1 (-1.92145) | -1 | -1 |
| G: -6289.33611 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.35580 HOMO: -7.37429 LUMO: 0.09252 factor:1 | 1 (-1.65399) | -1 | -1 |
| G: -6289.33611 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12556.39514 HOMO: -6.54434 LUMO: -0.39729 factor:1 | 1 (-2.69333) | -1 | -1 |
| G: -6289.33611 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12556.30681 HOMO: -7.35524 LUMO: 0.28028 factor:1 | 1 (-2.60500) | -1 | -1 |
| G: -6289.33611 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12556.17853 HOMO: -6.95523 LUMO: -0.86804 factor:1 | 1 (-2.47673) | -1 | -1 |
| G: -6289.33611 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.19373 HOMO: -6.63958 LUMO: -0.65307 factor:1 | 1 (-1.49192) | -1 | -1 |
| G: -6289.33611 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12553.87792 HOMO: -6.73482 LUMO: -0.67212 factor:1 | 1 (-0.17611) | -1 | -1 |
| G: -6289.33611 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.09156 HOMO: -6.37835 LUMO: -0.53606 factor:1 | 1 (-0.38975) | -1 | -1 |
| G: -6289.33611 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.24691 HOMO: -6.71849 LUMO: -0.61226 factor:1 | 1 (-0.54510) | -1 | -1 |
| G: -6289.33611 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.83445 HOMO: -6.68584 LUMO: -1.11022 factor:1 | 1 (-2.13264) | -1 | -1 |
| G: -6289.33611 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.80266 HOMO: -6.80285 LUMO: -0.79185 factor:1 | 1 (-2.10086) | -1 | -1 |
| G: -6289.33611 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.00401 HOMO: -7.14571 LUMO: -0.94696 factor:1 | 1 (-1.30220) | -1 | -1 |
| G: -6289.33611 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.69183 HOMO: -7.16204 LUMO: -0.66124 factor:1 | 1 (-1.99002) | -1 | -1 |
| G: -6289.33611 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.87652 HOMO: -6.54978 LUMO: -0.54967 factor:1 | 1 (-1.17472) | -1 | -1 |
| G: -6289.33611 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.90262 HOMO: -6.75114 LUMO: -0.70750 factor:1 | 1 (-1.20081) | -1 | -1 |
| G: -6289.33611 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.88136 HOMO: -7.22190 LUMO: 0.39184 factor:1 | 1 (-2.17955) | -1 | -1 |
| G: -6289.33611 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.09870 HOMO: -7.43959 LUMO: 0.30477 factor:1 | 1 (-1.39690) | -1 | -1 |
| G: -6289.33611 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.11990 HOMO: -6.87360 LUMO: -0.77552 factor:1 | 1 (-1.41809) | -1 | -1 |
| G: -6289.33611 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.23016 HOMO: -6.82734 LUMO: -0.59593 factor:1 | 1 (-1.52835) | -1 | -1 |
| G: -6727.83391 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12991.26024 HOMO: -6.65318 LUMO: -0.46259 factor:1 | -1 (0.93936) | -1 | -1 |
| G: -6727.83391 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12991.00976 HOMO: -7.05863 LUMO: -1.17009 factor:1 | -1 (1.18985) | -1 | -1 |
| G: -6727.83391 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12991.13880 HOMO: -6.57427 LUMO: -0.48708 factor:1 | -1 (1.06081) | -1 | -1 |
| G: -6727.83391 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12990.82383 HOMO: -6.60420 LUMO: -0.38096 factor:1 | -1 (1.37578) | -1 | -1 |
| G: -6727.83391 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12990.59914 HOMO: -6.72121 LUMO: -0.66668 factor:1 | -1 (1.60046) | -1 | -1 |
| G: -6727.83391 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12990.85749 HOMO: -6.52257 LUMO: -0.19320 factor:1 | -1 (1.34212) | -1 | -1 |
| G: -6727.83391 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12990.88976 HOMO: -6.28039 LUMO: -0.27211 factor:1 | -1 (1.30985) | -1 | -1 |
| G: -6727.83391 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12990.95806 HOMO: -6.71849 LUMO: -0.42722 factor:1 | -1 (1.24155) | -1 | -1 |
| G: -6727.83391 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12990.85215 HOMO: -6.27495 LUMO: 0.27756 factor:1 | -1 (1.34745) | -1 | -1 |
| G: -6727.83391 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12991.17102 HOMO: -6.21780 LUMO: 0.46531 factor:1 | -1 (1.02859) | -1 | -1 |
| G: -6727.83391 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12990.83561 HOMO: -6.52257 LUMO: -0.64491 factor:1 | -1 (1.36400) | -1 | -1 |
| G: -6727.83391 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12991.02775 HOMO: -6.73754 LUMO: 1.83133 factor:1 | -1 (1.17186) | -1 | -1 |
| G: -6727.83391 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12990.63471 HOMO: -6.67223 LUMO: 1.88847 factor:1 | -1 (1.56490) | -1 | -1 |
| G: -6727.83391 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12990.80219 HOMO: -6.82189 LUMO: 1.59187 factor:1 | -1 (1.39741) | -1 | -1 |
| G: -6727.83391 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12990.98786 HOMO: -6.43277 LUMO: 1.76330 factor:1 | -1 (1.21175) | -1 | -1 |
| G: -6727.83391 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12990.84347 HOMO: -6.48175 LUMO: 1.77962 factor:1 | -1 (1.35613) | -1 | -1 |
| G: -6727.83391 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12993.82026 HOMO: -6.50352 LUMO: 1.68438 factor:1 | 1 (-1.62066) | -1 | -1 |
| G: -6727.83391 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12993.33114 HOMO: -6.31576 LUMO: 2.03813 factor:1 | 1 (-1.13153) | -1 | -1 |
| G: -6727.83391 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12993.38417 HOMO: -6.27495 LUMO: 1.99459 factor:1 | 1 (-1.18457) | -1 | -1 |
| G: -6727.83391 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12993.53280 HOMO: -6.23957 LUMO: 2.17147 factor:1 | 1 (-1.33319) | -1 | -1 |
| G: -6727.83391 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12993.40551 HOMO: -6.78108 LUMO: 2.16875 factor:1 | 1 (-1.20590) | -1 | -1 |
| G: -6727.83391 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12993.41383 HOMO: -6.34297 LUMO: 2.10344 factor:1 | 1 (-1.21423) | -1 | -1 |
| G: -6727.83391 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12993.43702 HOMO: -6.30216 LUMO: 2.00004 factor:1 | 1 (-1.23741) | -1 | -1 |
| G: -6727.83391 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12993.32866 HOMO: -6.72665 LUMO: 2.09528 factor:1 | 1 (-1.12905) | -1 | -1 |
| G: -6727.83391 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12993.79060 HOMO: -6.86543 LUMO: 1.91568 factor:1 | 1 (-1.59100) | -1 | -1 |
| G: -6727.83391 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12993.27301 HOMO: -5.83956 LUMO: 1.89391 factor:1 | 1 (-1.07341) | -1 | -1 |
| G: -6727.83391 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12993.24926 HOMO: -6.42189 LUMO: 2.03269 factor:1 | 1 (-1.04965) | -1 | -1 |
| G: -6727.83391 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12992.94465 HOMO: -6.07630 LUMO: 1.80956 factor:1 | 1 (-0.74505) | -1 | -1 |
| G: -6727.83391 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12992.08826 HOMO: -6.43277 LUMO: 1.81772 factor:1 | -1 (0.11135) | -1 | -1 |
| G: -6727.83391 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12993.43424 HOMO: -7.03959 LUMO: 1.78779 factor:1 | 1 (-1.23464) | -1 | -1 |
| G: -6727.83391 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12993.31723 HOMO: -6.72121 LUMO: 2.29664 factor:1 | 1 (-1.11763) | -1 | -1 |
| G: -6727.83391 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12993.41081 HOMO: -6.62869 LUMO: 2.04630 factor:1 | 1 (-1.21121) | -1 | -1 |
| G: -6727.83391 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12992.00246 HOMO: -6.63958 LUMO: 1.84221 factor:1 | -1 (0.19715) | -1 | -1 |
| G: -6727.83391 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12992.89241 HOMO: -6.70761 LUMO: 1.67350 factor:1 | 1 (-0.69280) | -1 | -1 |
| G: -6727.83391 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12993.66072 HOMO: -6.00283 LUMO: 1.64357 factor:1 | 1 (-1.46112) | -1 | -1 |
| G: -6727.83391 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12993.11024 HOMO: -6.48719 LUMO: 1.70343 factor:1 | 1 (-0.91063) | -1 | -1 |
| G: -6727.83391 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12992.98642 HOMO: -6.13345 LUMO: 1.44492 factor:1 | 1 (-0.78682) | -1 | -1 |
| G: -6727.83391 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12993.20817 HOMO: -6.11168 LUMO: 1.70071 factor:1 | 1 (-1.00856) | -1 | -1 |
| G: -6727.83391 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12992.98593 HOMO: -6.09535 LUMO: 1.82316 factor:1 | 1 (-0.78633) | -1 | -1 |
| G: -6727.83391 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12993.19535 HOMO: -6.81101 LUMO: 1.63540 factor:1 | 1 (-0.99575) | -1 | -1 |
| G: -6727.83391 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12993.06724 HOMO: -6.80013 LUMO: 2.12249 factor:1 | 1 (-0.86764) | -1 | -1 |
| G: -6727.83391 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12993.17954 HOMO: -6.48447 LUMO: 1.94561 factor:1 | 1 (-0.97994) | -1 | -1 |
| G: -6727.83391 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12993.11247 HOMO: -6.72393 LUMO: 2.06534 factor:1 | 1 (-0.91286) | -1 | -1 |
| G: -6727.83391 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12993.62935 HOMO: -6.34570 LUMO: 1.98915 factor:1 | 1 (-1.42974) | -1 | -1 |
| G: -6727.83391 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12993.54472 HOMO: -6.31304 LUMO: 1.87759 factor:1 | 1 (-1.34511) | -1 | -1 |
| G: -6727.83391 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12993.28327 HOMO: -6.77564 LUMO: 1.81228 factor:1 | 1 (-1.08367) | -1 | -1 |
| G: -6727.83391 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12993.34336 HOMO: -6.58516 LUMO: 2.34834 factor:1 | 1 (-1.14375) | -1 | -1 |
| G: -6727.83391 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12993.11285 HOMO: -6.68040 LUMO: 2.20412 factor:1 | 1 (-0.91324) | -1 | -1 |
| G: -6727.83391 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12992.65706 HOMO: -6.20964 LUMO: 2.17147 factor:1 | 1 (-0.45745) | -1 | -1 |
| G: -6727.83391 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12993.11690 HOMO: -6.54706 LUMO: 2.03813 factor:1 | 1 (-0.91730) | -1 | -1 |
| G: -6727.83391 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12993.00585 HOMO: -6.54162 LUMO: 2.17419 factor:1 | 1 (-0.80625) | -1 | -1 |
| G: -6727.83391 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12993.00974 HOMO: -6.75659 LUMO: 2.22589 factor:1 | 1 (-0.81014) | -1 | -1 |
| G: -6727.83391 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12993.59245 HOMO: -6.59604 LUMO: 2.59325 factor:1 | 1 (-1.39284) | -1 | -1 |
| G: -6727.83391 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12993.29840 HOMO: -6.11712 LUMO: 2.02181 factor:1 | 1 (-1.09880) | -1 | -1 |
| G: -6727.83391 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12993.36477 HOMO: -6.63141 LUMO: 2.09256 factor:1 | 1 (-1.16516) | -1 | -1 |
| G: -6727.83391 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12993.29187 HOMO: -6.61781 LUMO: 1.86126 factor:1 | 1 (-1.09227) | -1 | -1 |
| G: -6727.83391 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12992.96313 HOMO: -6.63958 LUMO: 1.77146 factor:1 | 1 (-0.76352) | -1 | -1 |
| G: -6727.83391 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12992.07743 HOMO: -6.60420 LUMO: 1.54561 factor:1 | -1 (0.12218) | -1 | -1 |
| G: -6727.83391 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12993.25622 HOMO: -6.52529 LUMO: 2.05174 factor:1 | 1 (-1.05662) | -1 | -1 |
| G: -6727.83391 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12993.07021 HOMO: -6.80285 LUMO: 2.13609 factor:1 | 1 (-0.87060) | -1 | -1 |
| G: -6727.83391 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12993.29606 HOMO: -6.51168 LUMO: 2.25855 factor:1 | 1 (-1.09646) | -1 | -1 |
| G: -6727.83391 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12993.26376 HOMO: -6.64774 LUMO: 2.46263 factor:1 | 1 (-1.06416) | -1 | -1 |
| G: -6727.83391 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12993.29799 HOMO: -6.40828 LUMO: 1.99732 factor:1 | 1 (-1.09839) | -1 | -1 |
| G: -6727.83391 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12992.99954 HOMO: -5.97562 LUMO: 1.56465 factor:1 | 1 (-0.79993) | -1 | -1 |
| G: -6727.83391 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12993.00226 HOMO: -6.75659 LUMO: 2.23405 factor:1 | 1 (-0.80265) | -1 | -1 |
| G: -6727.83391 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12992.84193 HOMO: -6.68584 LUMO: 2.09528 factor:1 | 1 (-0.64232) | -1 | -1 |
| G: -6727.83391 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12991.03578 HOMO: -6.86543 LUMO: 1.95106 factor:1 | -1 (1.16383) | -1 | -1 |
| G: -6727.83391 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12992.69330 HOMO: -6.47359 LUMO: 1.82316 factor:1 | 1 (-0.49370) | -1 | -1 |
| G: -6727.83391 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12991.86137 HOMO: -6.87632 LUMO: 2.08439 factor:1 | -1 (0.33824) | -1 | -1 |
| G: -6727.83391 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12992.75507 HOMO: -6.33753 LUMO: 2.16603 factor:1 | 1 (-0.55547) | -1 | -1 |
| G: -6727.83391 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12993.18063 HOMO: -6.92258 LUMO: 1.72248 factor:1 | 1 (-0.98102) | -1 | -1 |
| G: -6727.83391 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12993.27916 HOMO: -6.62597 LUMO: 2.10344 factor:1 | 1 (-1.07956) | -1 | -1 |
| G: -6727.83391 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12993.12836 HOMO: -6.63141 LUMO: 1.94017 factor:1 | 1 (-0.92875) | -1 | -1 |
| G: -6727.83391 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12991.14900 HOMO: -6.48447 LUMO: 1.91840 factor:1 | -1 (1.05060) | -1 | -1 |
| G: -6727.83391 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12993.09715 HOMO: -6.41372 LUMO: 1.61364 factor:1 | 1 (-0.89754) | -1 | -1 |
| G: -6727.83391 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12993.17005 HOMO: -6.37291 LUMO: 1.79051 factor:1 | 1 (-0.97044) | -1 | -1 |
| G: -6727.83391 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12993.44227 HOMO: -6.13073 LUMO: 1.77962 factor:1 | 1 (-1.24266) | -1 | -1 |
| G: -6727.83391 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12993.27769 HOMO: -6.13073 LUMO: 1.98915 factor:1 | 1 (-1.07809) | -1 | -1 |
| G: -6727.83391 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12993.41508 HOMO: -6.44094 LUMO: 1.58370 factor:1 | 1 (-1.21548) | -1 | -1 |
| G: -6727.83391 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12993.06185 HOMO: -6.87087 LUMO: -0.82995 factor:1 | 1 (-0.86225) | -1 | -1 |
| G: -6727.83391 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12993.03415 HOMO: -6.67223 LUMO: 1.08029 factor:1 | 1 (-0.83455) | -1 | -1 |
| G: -6727.83391 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12993.13391 HOMO: -6.82462 LUMO: 0.91702 factor:1 | 1 (-0.93430) | -1 | -1 |
| G: -6727.83391 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12990.99431 HOMO: -6.65863 LUMO: 1.52656 factor:1 | -1 (1.20530) | -1 | -1 |
| G: -6727.83391 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12992.84332 HOMO: -6.78924 LUMO: 0.86260 factor:1 | 1 (-0.64371) | -1 | -1 |
| G: -6727.83391 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12992.05378 HOMO: -6.68584 LUMO: 0.94424 factor:1 | -1 (0.14583) | -1 | -1 |
| G: -6727.83391 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12990.96519 HOMO: -6.58788 LUMO: 1.00138 factor:1 | -1 (1.23442) | -1 | -1 |
| G: -6727.83391 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12991.02495 HOMO: -6.79740 LUMO: 0.91430 factor:1 | -1 (1.17466) | -1 | -1 |
| G: -6727.83391 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12993.10591 HOMO: -6.67223 LUMO: 0.80274 factor:1 | 1 (-0.90630) | -1 | -1 |
| G: -6727.83391 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12992.31594 HOMO: -6.95251 LUMO: 0.90614 factor:1 | 1 (-0.11633) | -1 | -1 |
| G: -6727.83391 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12993.09015 HOMO: -7.19469 LUMO: 1.34152 factor:1 | 1 (-0.89055) | -1 | -1 |
| G: -6727.83391 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12993.05407 HOMO: -6.59332 LUMO: -0.76464 factor:1 | 1 (-0.85446) | -1 | -1 |
| G: -6727.83391 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12993.55144 HOMO: -6.77564 LUMO: -0.90886 factor:1 | 1 (-1.35183) | -1 | -1 |
| G: -6727.83391 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12992.24491 HOMO: -6.57971 LUMO: -0.41633 factor:1 | 1 (-0.04531) | -1 | -1 |
| G: -6727.83391 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12992.36192 HOMO: -6.68856 LUMO: -0.58232 factor:1 | 1 (-0.16232) | -1 | -1 |
| G: -6727.83391 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12993.44853 HOMO: -6.87087 LUMO: -0.71022 factor:1 | 1 (-1.24892) | -1 | -1 |
| G: -6727.83391 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12992.65480 HOMO: -6.67767 LUMO: -0.74559 factor:1 | 1 (-0.45519) | -1 | -1 |
| G: -6727.83391 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12992.41920 HOMO: -6.68040 LUMO: -0.65307 factor:1 | 1 (-0.21960) | -1 | -1 |
| G: -6727.83391 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12993.13551 HOMO: -6.32937 LUMO: 0.80274 factor:1 | 1 (-0.93591) | -1 | -1 |
| G: -6727.83391 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12993.06996 HOMO: -6.29671 LUMO: 0.82723 factor:1 | 1 (-0.87036) | -1 | -1 |
| G: -6727.83391 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12993.50573 HOMO: -6.67767 LUMO: 0.59321 factor:1 | 1 (-1.30612) | -1 | -1 |
| G: -6727.83391 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12992.97772 HOMO: -6.77836 LUMO: 0.50341 factor:1 | 1 (-0.77811) | -1 | -1 |
| G: -6727.83391 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12992.87782 HOMO: -6.61781 LUMO: 0.42450 factor:1 | 1 (-0.67822) | -1 | -1 |
| G: -6727.83391 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12993.63122 HOMO: -6.83278 LUMO: 0.39457 factor:1 | 1 (-1.43162) | -1 | -1 |
| G: -6727.83391 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12993.33084 HOMO: -6.56883 LUMO: 0.64219 factor:1 | 1 (-1.13123) | -1 | -1 |
| G: -6727.83391 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12993.17998 HOMO: -6.71577 LUMO: 0.40001 factor:1 | 1 (-0.98037) | -1 | -1 |
| G: -6727.83391 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12993.17105 HOMO: -6.86543 LUMO: -0.74287 factor:1 | 1 (-0.97145) | -1 | -1 |
| G: -6727.83391 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12990.46842 HOMO: -6.68584 LUMO: -0.69389 factor:1 | -1 (1.73119) | -1 | -1 |
| G: -6727.83391 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12991.77124 HOMO: -6.61237 LUMO: -0.48980 factor:1 | -1 (0.42836) | -1 | -1 |
| G: -6727.83391 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12992.74949 HOMO: -6.80285 LUMO: -0.58232 factor:1 | 1 (-0.54989) | -1 | -1 |
| G: -6727.83391 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12991.97919 HOMO: -6.88992 LUMO: -0.70205 factor:1 | -1 (0.22041) | -1 | -1 |
| G: -6727.83391 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12992.92392 HOMO: -6.95251 LUMO: -0.71838 factor:1 | 1 (-0.72431) | -1 | -1 |
| G: -6727.83391 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12992.77167 HOMO: -7.52123 LUMO: 0.27211 factor:1 | 1 (-0.57206) | -1 | -1 |
| G: -6727.83391 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12992.54832 HOMO: -6.76747 LUMO: -0.74015 factor:1 | 1 (-0.34871) | -1 | -1 |
| G: -6727.83391 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12992.08268 HOMO: -6.55250 LUMO: -0.49797 factor:1 | -1 (0.11693) | -1 | -1 |
| G: -6727.83391 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12991.77650 HOMO: -6.50896 LUMO: -0.46804 factor:1 | -1 (0.42311) | -1 | -1 |
| G: -6727.83391 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12992.49330 HOMO: -7.45320 LUMO: 0.08436 factor:1 | 1 (-0.29369) | -1 | -1 |
| G: -6727.83391 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12992.24053 HOMO: -6.82462 LUMO: -0.70477 factor:1 | 1 (-0.04093) | -1 | -1 |
| G: -6727.83391 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12993.12762 HOMO: -6.57155 LUMO: -0.43538 factor:1 | 1 (-0.92802) | -1 | -1 |
| G: -6727.83391 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12993.64965 HOMO: -6.72665 LUMO: -0.55239 factor:1 | 1 (-1.45004) | -1 | -1 |
| G: -6727.83391 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12993.01551 HOMO: -7.05319 LUMO: -1.08573 factor:1 | 1 (-0.81591) | -1 | -1 |
| G: -6727.83391 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12990.76614 HOMO: -6.56067 LUMO: -0.45715 factor:1 | -1 (1.43347) | -1 | -1 |
| G: -6727.83391 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12992.87834 HOMO: -6.76475 LUMO: -0.53879 factor:1 | 1 (-0.67873) | -1 | -1 |
| G: -6727.83391 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12993.01826 HOMO: -6.67223 LUMO: -0.45987 factor:1 | 1 (-0.81865) | -1 | -1 |
| G: -6727.83391 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12990.72959 HOMO: -6.44094 LUMO: -0.72110 factor:1 | -1 (1.47001) | -1 | -1 |
| G: -6727.83391 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12992.02241 HOMO: -6.66951 LUMO: -0.67756 factor:1 | -1 (0.17720) | -1 | -1 |
| G: -6727.83391 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12992.57039 HOMO: -6.69400 LUMO: -0.62858 factor:1 | 1 (-0.37078) | -1 | -1 |
| G: -6727.83391 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12991.61799 HOMO: -6.51985 LUMO: -0.37007 factor:1 | -1 (0.58162) | -1 | -1 |
| G: -6727.83391 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12992.67488 HOMO: -5.98378 LUMO: 0.78641 factor:1 | 1 (-0.47527) | -1 | -1 |
| G: -6727.83391 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12991.78284 HOMO: -6.11440 LUMO: 0.71294 factor:1 | -1 (0.41677) | -1 | -1 |
| G: -6727.83391 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12992.97494 HOMO: -6.45182 LUMO: 0.63947 factor:1 | 1 (-0.77533) | -1 | -1 |
| G: -6727.83391 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12992.06281 HOMO: -6.78924 LUMO: 0.37007 factor:1 | -1 (0.13679) | -1 | -1 |
| G: -6727.83391 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12990.93988 HOMO: -6.63686 LUMO: 0.54423 factor:1 | -1 (1.25972) | -1 | -1 |
| G: -6727.83391 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12991.76104 HOMO: -6.66679 LUMO: 0.48708 factor:1 | -1 (0.43857) | -1 | -1 |
| G: -6727.83391 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12991.88801 HOMO: -6.81917 LUMO: 0.31021 factor:1 | -1 (0.31160) | -1 | -1 |
| G: -6727.83391 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12993.23443 HOMO: -6.28583 LUMO: 0.44899 factor:1 | 1 (-1.03482) | -1 | -1 |
| G: -6727.83391 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12992.35153 HOMO: -6.61237 LUMO: 0.49525 factor:1 | 1 (-0.15192) | -1 | -1 |
| G: -6727.83391 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12993.11356 HOMO: -7.08857 LUMO: 0.38368 factor:1 | 1 (-0.91395) | -1 | -1 |
| G: -6727.83391 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12993.20670 HOMO: -6.53890 LUMO: -0.68845 factor:1 | 1 (-1.00709) | -1 | -1 |
| G: -6727.83391 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12993.31106 HOMO: -6.56611 LUMO: -0.66396 factor:1 | 1 (-1.11145) | -1 | -1 |
| G: -6727.83391 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12993.33119 HOMO: -6.04909 LUMO: -0.59865 factor:1 | 1 (-1.13159) | -1 | -1 |
| G: -6727.83391 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12993.19456 HOMO: -6.74842 LUMO: -0.77825 factor:1 | 1 (-0.99496) | -1 | -1 |
| G: -6727.83391 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12993.02313 HOMO: -6.82462 LUMO: -0.61498 factor:1 | 1 (-0.82353) | -1 | -1 |
| G: -6727.83391 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12993.10030 HOMO: -7.40694 LUMO: 0.32926 factor:1 | 1 (-0.90070) | -1 | -1 |
| G: -6727.83391 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12992.79978 HOMO: -6.80557 LUMO: -0.57416 factor:1 | 1 (-0.60017) | -1 | -1 |
| G: -6727.83391 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12993.03954 HOMO: -6.76747 LUMO: -0.67484 factor:1 | 1 (-0.83993) | -1 | -1 |
| G: -6727.83391 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12992.93401 HOMO: -7.23279 LUMO: 0.48980 factor:1 | 1 (-0.73441) | -1 | -1 |
| G: -6727.83391 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12992.31057 HOMO: -6.62869 LUMO: -0.24762 factor:1 | 1 (-0.11097) | -1 | -1 |
| G: -6727.83391 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12992.81848 HOMO: -6.65863 LUMO: -0.28028 factor:1 | 1 (-0.61887) | -1 | -1 |
| G: -6727.83391 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12993.14000 HOMO: -6.50352 LUMO: -0.44899 factor:1 | 1 (-0.94040) | -1 | -1 |
| G: -6727.83391 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12992.60623 HOMO: -6.62053 LUMO: -0.88437 factor:1 | 1 (-0.40662) | -1 | -1 |
| G: -6727.83391 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12991.90210 HOMO: -6.73754 LUMO: -0.77825 factor:1 | -1 (0.29750) | -1 | -1 |
| G: -6727.83391 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12993.60796 HOMO: -7.24639 LUMO: 0.35647 factor:1 | 1 (-1.40835) | -1 | -1 |
| G: -6727.83391 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12992.70206 HOMO: -6.46270 LUMO: -0.48164 factor:1 | 1 (-0.50246) | -1 | -1 |
| G: -6727.83391 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12993.02501 HOMO: -6.14161 LUMO: -0.66396 factor:1 | 1 (-0.82540) | -1 | -1 |
| G: -6727.83391 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12993.36831 HOMO: -6.63414 LUMO: 1.51295 factor:1 | 1 (-1.16870) | -1 | -1 |
| G: -6727.83391 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12993.01083 HOMO: -6.52529 LUMO: 1.65989 factor:1 | 1 (-0.81123) | -1 | -1 |
| G: -6727.83391 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12993.01415 HOMO: -6.63686 LUMO: 1.64629 factor:1 | 1 (-0.81455) | -1 | -1 |
| G: -6727.83391 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12993.11132 HOMO: -6.49808 LUMO: 1.60003 factor:1 | 1 (-0.91172) | -1 | -1 |
| G: -6727.83391 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12993.13007 HOMO: -6.85183 LUMO: 1.96194 factor:1 | 1 (-0.93047) | -1 | -1 |
| G: -6727.83391 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12993.36570 HOMO: -6.90081 LUMO: 1.82316 factor:1 | 1 (-1.16609) | -1 | -1 |
| G: -6727.83391 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12992.65610 HOMO: -6.20147 LUMO: 1.95106 factor:1 | 1 (-0.45650) | -1 | -1 |
| G: -6727.83391 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12991.70724 HOMO: -7.05047 LUMO: 1.94289 factor:1 | -1 (0.49236) | -1 | -1 |
| G: -6727.83391 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12992.78435 HOMO: -6.11440 LUMO: 1.83949 factor:1 | 1 (-0.58475) | -1 | -1 |
| G: -6727.83391 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12991.81720 HOMO: -6.65046 LUMO: 1.59187 factor:1 | -1 (0.38240) | -1 | -1 |
| G: -6727.83391 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12993.11312 HOMO: -6.81917 LUMO: 2.41365 factor:1 | 1 (-0.91351) | -1 | -1 |
| G: -6727.83391 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12991.24718 HOMO: -6.40284 LUMO: 2.48984 factor:1 | -1 (0.95243) | -1 | -1 |
| G: -6727.83391 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12993.01821 HOMO: -7.04775 LUMO: 2.31025 factor:1 | 1 (-0.81860) | -1 | -1 |
| G: -6727.83391 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12992.96876 HOMO: -6.64774 LUMO: 2.20140 factor:1 | 1 (-0.76916) | -1 | -1 |
| G: -6727.83391 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12992.69676 HOMO: -6.72393 LUMO: 2.28304 factor:1 | 1 (-0.49715) | -1 | -1 |
| G: -6727.83391 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12993.08792 HOMO: -6.35114 LUMO: 1.84765 factor:1 | 1 (-0.88832) | -1 | -1 |
| G: -6727.83391 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12991.02799 HOMO: -6.41100 LUMO: 1.74697 factor:1 | -1 (1.17161) | -1 | -1 |
| G: -6727.83391 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12992.87445 HOMO: -6.34297 LUMO: 1.55921 factor:1 | 1 (-0.67484) | -1 | -1 |
| G: -6727.83391 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12992.67115 HOMO: -6.31848 LUMO: 1.67622 factor:1 | 1 (-0.47155) | -1 | -1 |
| G: -6727.83391 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12992.87434 HOMO: -6.50896 LUMO: 2.02725 factor:1 | 1 (-0.67473) | -1 | -1 |
| G: -6727.83391 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12992.77603 HOMO: -6.28583 LUMO: 2.00548 factor:1 | 1 (-0.57642) | -1 | -1 |
| G: -6727.83391 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12992.49044 HOMO: -6.67495 LUMO: 1.92384 factor:1 | 1 (-0.29084) | -1 | -1 |
| G: -6727.83391 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12992.94536 HOMO: -6.17154 LUMO: 2.39732 factor:1 | 1 (-0.74576) | -1 | -1 |
| G: -6727.83391 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12993.10311 HOMO: -6.84911 LUMO: 2.24766 factor:1 | 1 (-0.90350) | -1 | -1 |
| G: -6727.83391 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12993.23467 HOMO: -6.77564 LUMO: 2.38372 factor:1 | 1 (-1.03507) | -1 | -1 |
| G: -6727.83391 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12992.62639 HOMO: -6.18243 LUMO: 2.40821 factor:1 | 1 (-0.42678) | -1 | -1 |
| G: -6727.83391 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12991.58721 HOMO: -6.40828 LUMO: 2.22589 factor:1 | -1 (0.61239) | -1 | -1 |
| G: -6727.83391 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12992.68854 HOMO: -6.74570 LUMO: 1.88303 factor:1 | 1 (-0.48893) | -1 | -1 |
| G: -6727.83391 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12991.88932 HOMO: -6.29944 LUMO: 2.05174 factor:1 | -1 (0.31029) | -1 | -1 |
| G: -6727.83391 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12992.61099 HOMO: -7.00693 LUMO: 2.16331 factor:1 | 1 (-0.41138) | -1 | -1 |
| G: -6727.83391 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12991.88948 HOMO: -6.89537 LUMO: 2.19596 factor:1 | -1 (0.31013) | -1 | -1 |
| G: -6727.83391 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12993.00833 HOMO: -6.72665 LUMO: 2.03813 factor:1 | 1 (-0.80872) | -1 | -1 |
| G: -6727.83391 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12993.15592 HOMO: -6.69944 LUMO: 2.36467 factor:1 | 1 (-0.95632) | -1 | -1 |
| G: -6727.83391 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12993.22126 HOMO: -6.92802 LUMO: 1.72792 factor:1 | 1 (-1.02165) | -1 | -1 |
| G: -6727.83391 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12993.50766 HOMO: -6.12256 LUMO: 1.85310 factor:1 | 1 (-1.30805) | -1 | -1 |
| G: -6727.83391 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12993.51830 HOMO: -6.70489 LUMO: 2.20956 factor:1 | 1 (-1.31869) | -1 | -1 |
| G: -6727.83391 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12992.71777 HOMO: -6.94707 LUMO: 1.81500 factor:1 | 1 (-0.51816) | -1 | -1 |
| G: -6727.83391 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12992.66895 HOMO: -6.39468 LUMO: 1.79051 factor:1 | 1 (-0.46934) | -1 | -1 |
| G: -6727.83391 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12992.93927 HOMO: -6.69128 LUMO: 2.03813 factor:1 | 1 (-0.73966) | -1 | -1 |
| G: -6727.83391 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12992.96441 HOMO: -6.55250 LUMO: 2.00548 factor:1 | 1 (-0.76480) | -1 | -1 |
| G: -6727.83391 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12993.05720 HOMO: -6.24773 LUMO: 2.09256 factor:1 | 1 (-0.85759) | -1 | -1 |
| G: -6727.83391 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12992.96289 HOMO: -6.85727 LUMO: 1.70071 factor:1 | 1 (-0.76328) | -1 | -1 |
| G: -6727.83391 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12993.13761 HOMO: -6.71305 LUMO: 1.72520 factor:1 | 1 (-0.93800) | -1 | -1 |
| G: -6727.83391 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12993.08324 HOMO: -6.81101 LUMO: 2.15514 factor:1 | 1 (-0.88364) | -1 | -1 |
| G: -6727.83391 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12993.07402 HOMO: -6.93618 LUMO: 1.75513 factor:1 | 1 (-0.87441) | -1 | -1 |
| G: -6727.83391 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12993.14670 HOMO: -6.63686 LUMO: 2.09800 factor:1 | 1 (-0.94709) | -1 | -1 |
| G: -6727.83391 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12992.95418 HOMO: -6.98244 LUMO: 1.72520 factor:1 | 1 (-0.75457) | -1 | -1 |
| G: -6727.83391 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12992.95040 HOMO: -6.37019 LUMO: 2.35923 factor:1 | 1 (-0.75079) | -1 | -1 |
| G: -6727.83391 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12993.12912 HOMO: -6.55794 LUMO: 2.12521 factor:1 | 1 (-0.92951) | -1 | -1 |
| G: -6727.83391 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12993.10234 HOMO: -6.45998 LUMO: 1.93201 factor:1 | 1 (-0.90274) | -1 | -1 |
| G: -6727.83391 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12993.22684 HOMO: -6.71033 LUMO: 1.58370 factor:1 | 1 (-1.02723) | -1 | -1 |
| G: -6727.83391 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12991.83342 HOMO: -6.67223 LUMO: 1.52928 factor:1 | -1 (0.36618) | -1 | -1 |
| G: -6727.83391 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12992.73692 HOMO: -6.72121 LUMO: 1.33608 factor:1 | 1 (-0.53732) | -1 | -1 |
| G: -6727.83391 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12993.36311 HOMO: -6.89264 LUMO: 2.08983 factor:1 | 1 (-1.16350) | -1 | -1 |
| G: -6727.83391 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12993.15456 HOMO: -6.31032 LUMO: 2.24766 factor:1 | 1 (-0.95496) | -1 | -1 |
| G: -6727.83391 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12991.96494 HOMO: -6.79740 LUMO: 2.09528 factor:1 | -1 (0.23467) | -1 | -1 |
| G: -6727.83391 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12992.24483 HOMO: -6.78108 LUMO: 2.15786 factor:1 | 1 (-0.04523) | -1 | -1 |
| G: -6727.83391 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12992.74364 HOMO: -6.50896 LUMO: 2.15786 factor:1 | 1 (-0.54404) | -1 | -1 |
| G: -6727.83391 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12993.31473 HOMO: -6.56067 LUMO: 2.24494 factor:1 | 1 (-1.11512) | -1 | -1 |
| G: -6727.83391 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12992.81997 HOMO: -6.72938 LUMO: 2.24494 factor:1 | 1 (-0.62037) | -1 | -1 |
| G: -6727.83391 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12993.18172 HOMO: -6.40556 LUMO: 1.58642 factor:1 | 1 (-0.98211) | -1 | -1 |
| G: -6727.83391 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12991.93666 HOMO: -6.63141 LUMO: 1.66262 factor:1 | -1 (0.26294) | -1 | -1 |
| G: -6727.83391 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12992.02654 HOMO: -6.97156 LUMO: 2.23678 factor:1 | -1 (0.17306) | -1 | -1 |
| G: -6727.83391 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12992.69602 HOMO: -6.86271 LUMO: 1.91296 factor:1 | 1 (-0.49642) | -1 | -1 |
| G: -6727.83391 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12992.91317 HOMO: -6.50624 LUMO: 1.89119 factor:1 | 1 (-0.71356) | -1 | -1 |
| G: -6727.83391 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12992.66057 HOMO: -6.70761 LUMO: 1.56193 factor:1 | 1 (-0.46096) | -1 | -1 |
| G: -6727.83391 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12992.14464 HOMO: -6.60420 LUMO: 1.79595 factor:1 | -1 (0.05497) | -1 | -1 |
| G: -6727.83391 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12993.40747 HOMO: -6.85727 LUMO: 2.26943 factor:1 | 1 (-1.20786) | -1 | -1 |
| G: -6727.83391 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12992.72620 HOMO: -6.23413 LUMO: 1.91024 factor:1 | 1 (-0.52659) | -1 | -1 |
| G: -6727.83391 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12993.27057 HOMO: -6.84366 LUMO: 2.01364 factor:1 | 1 (-1.07096) | -1 | -1 |
| G: -6727.83391 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12992.74313 HOMO: -6.63414 LUMO: 2.54971 factor:1 | 1 (-0.54352) | -1 | -1 |
| G: -6727.83391 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12992.51137 HOMO: -6.52257 LUMO: 2.42998 factor:1 | 1 (-0.31176) | -1 | -1 |
| G: -6727.83391 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12992.96044 HOMO: -6.61509 LUMO: 2.31297 factor:1 | 1 (-0.76083) | -1 | -1 |
| G: -6727.83391 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12992.61692 HOMO: -6.45998 LUMO: 2.23405 factor:1 | 1 (-0.41731) | -1 | -1 |
| G: -6727.83391 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12993.48921 HOMO: -6.86271 LUMO: 2.22317 factor:1 | 1 (-1.28960) | -1 | -1 |
| G: -6727.83391 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12992.50769 HOMO: -6.84366 LUMO: 2.11432 factor:1 | 1 (-0.30809) | -1 | -1 |
| G: -6727.83391 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12990.37307 HOMO: -6.85999 LUMO: 2.44902 factor:1 | -1 (1.82654) | -1 | -1 |
| G: -6727.83391 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12992.87396 HOMO: -6.73482 LUMO: 1.93745 factor:1 | 1 (-0.67435) | -1 | -1 |
| G: -6727.83391 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12992.96670 HOMO: -6.91441 LUMO: 2.32385 factor:1 | 1 (-0.76709) | -1 | -1 |
| G: -6727.83391 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12992.62146 HOMO: -6.16066 LUMO: 2.26399 factor:1 | 1 (-0.42186) | -1 | -1 |
| G: -6727.83391 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12991.69704 HOMO: -6.71305 LUMO: 2.38644 factor:1 | -1 (0.50257) | -1 | -1 |
| G: -6727.42770 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12991.26024 HOMO: -7.08312 LUMO: 2.01636 factor:1 | -1 (0.53315) | 1 | 1 |
| G: -6727.42770 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12991.00976 HOMO: -6.15249 LUMO: 1.90752 factor:1 | -1 (0.78363) | -1 | -1 |
| G: -6727.42770 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12991.13880 HOMO: -6.83006 LUMO: 2.25855 factor:1 | -1 (0.65460) | -1 | -1 |
| G: -6727.42770 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12990.82383 HOMO: -6.77836 LUMO: 2.24766 factor:1 | -1 (0.96957) | -1 | -1 |
| G: -6727.42770 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12990.59914 HOMO: -6.66951 LUMO: 2.35923 factor:1 | -1 (1.19425) | -1 | -1 |
| G: -6727.42770 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12990.85749 HOMO: -6.68312 LUMO: 2.30208 factor:1 | -1 (0.93591) | -1 | -1 |
| G: -6727.42770 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12990.88976 HOMO: -6.49808 LUMO: 2.49801 factor:1 | -1 (0.90364) | -1 | -1 |
| G: -6727.42770 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12990.95806 HOMO: -6.62325 LUMO: 1.89935 factor:1 | -1 (0.83534) | -1 | -1 |
| G: -6727.42770 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12990.85215 HOMO: -6.80829 LUMO: 1.91296 factor:1 | -1 (0.94124) | -1 | -1 |
| G: -6727.42770 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12991.17102 HOMO: -6.64230 LUMO: 2.13065 factor:1 | -1 (0.62238) | -1 | -1 |
| G: -6727.42770 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12990.83561 HOMO: -6.40556 LUMO: 1.83949 factor:1 | -1 (0.95779) | -1 | -1 |
| G: -6727.42770 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12991.02775 HOMO: -6.48175 LUMO: 1.72248 factor:1 | -1 (0.76565) | -1 | -1 |
| G: -6727.42770 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12990.63471 HOMO: -6.61781 LUMO: 2.11432 factor:1 | -1 (1.15869) | -1 | -1 |
| G: -6727.42770 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12990.80219 HOMO: -6.34570 LUMO: 2.22317 factor:1 | -1 (0.99120) | -1 | -1 |
| G: -6727.42770 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12990.98786 HOMO: -7.00149 LUMO: 1.80139 factor:1 | -1 (0.80554) | -1 | -1 |
| G: -6727.42770 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12990.84347 HOMO: -6.66951 LUMO: 2.13065 factor:1 | -1 (0.94992) | -1 | -1 |
| G: -6727.42770 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12993.82026 HOMO: -6.54434 LUMO: 2.20140 factor:1 | 1 (-2.02687) | -1 | -1 |
| G: -6727.42770 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12993.33114 HOMO: -6.67767 LUMO: 2.02997 factor:1 | 1 (-1.53774) | -1 | -1 |
| G: -6727.42770 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12993.38417 HOMO: -6.49536 LUMO: 2.42998 factor:1 | 1 (-1.59078) | -1 | -1 |
| G: -6727.42770 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12993.53280 HOMO: -6.70761 LUMO: 2.71025 factor:1 | 1 (-1.73941) | -1 | -1 |
| G: -6727.42770 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12993.40551 HOMO: -6.62869 LUMO: 2.11160 factor:1 | 1 (-1.61211) | -1 | -1 |
| G: -6727.42770 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12993.41383 HOMO: -6.61781 LUMO: 2.24494 factor:1 | 1 (-1.62044) | -1 | -1 |
| G: -6727.42770 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12993.43702 HOMO: -6.66135 LUMO: 2.20956 factor:1 | 1 (-1.64362) | -1 | -1 |
| G: -6727.42770 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12993.32866 HOMO: -6.95523 LUMO: 2.03813 factor:1 | 1 (-1.53527) | -1 | -1 |
| G: -6727.42770 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12993.79060 HOMO: -7.11578 LUMO: 2.41365 factor:1 | 1 (-1.99721) | 1 | 1 |
| G: -6727.42770 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12993.27301 HOMO: -6.99061 LUMO: 2.13881 factor:1 | 1 (-1.47962) | -1 | -1 |
| G: -6727.42770 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12993.24926 HOMO: -6.43277 LUMO: 2.01364 factor:1 | 1 (-1.45586) | -1 | -1 |
| G: -6727.42770 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12992.94465 HOMO: -6.79196 LUMO: 2.04358 factor:1 | 1 (-1.15126) | -1 | -1 |
| G: -6727.42770 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12992.08826 HOMO: -7.08584 LUMO: 1.99732 factor:1 | 1 (-0.29486) | 1 | 1 |
| G: -6727.42770 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12993.43424 HOMO: -6.46815 LUMO: 2.29936 factor:1 | 1 (-1.64085) | -1 | -1 |
| G: -6727.42770 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12993.31723 HOMO: -6.78108 LUMO: 1.93745 factor:1 | 1 (-1.52384) | -1 | -1 |
| G: -6727.42770 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12993.41081 HOMO: -6.43277 LUMO: 1.80956 factor:1 | 1 (-1.61742) | -1 | -1 |
| G: -6727.42770 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12992.00246 HOMO: -6.71577 LUMO: -0.81090 factor:1 | 1 (-0.20907) | -1 | -1 |
| G: -6727.42770 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12992.89241 HOMO: -7.14027 LUMO: -0.68028 factor:1 | 1 (-1.09901) | -1 | -1 |
| G: -6727.42770 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12993.66072 HOMO: -7.03414 LUMO: -0.69661 factor:1 | 1 (-1.86733) | -1 | -1 |
| G: -6727.42770 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12993.11024 HOMO: -6.64502 LUMO: -0.47348 factor:1 | 1 (-1.31684) | -1 | -1 |
| G: -6727.42770 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12992.98642 HOMO: -6.60692 LUMO: 2.12793 factor:1 | 1 (-1.19303) | -1 | -1 |
| G: -6727.42770 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12993.20817 HOMO: -6.66407 LUMO: 1.94561 factor:1 | 1 (-1.41477) | -1 | -1 |
| G: -6727.42770 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12992.98593 HOMO: -7.10217 LUMO: 1.92384 factor:1 | 1 (-1.19254) | 1 | 1 |
| G: -6727.42770 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12993.19535 HOMO: -6.84094 LUMO: 1.66534 factor:1 | 1 (-1.40196) | -1 | -1 |
| G: -6727.42770 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12993.06724 HOMO: -6.93618 LUMO: 2.13065 factor:1 | 1 (-1.27385) | -1 | -1 |
| G: -6727.42770 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12993.17954 HOMO: -6.60692 LUMO: 2.20684 factor:1 | 1 (-1.38615) | -1 | -1 |
| G: -6727.42770 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12993.11247 HOMO: -6.85727 LUMO: 2.19324 factor:1 | 1 (-1.31907) | -1 | -1 |
| G: -6727.42770 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12993.62935 HOMO: -6.31032 LUMO: 1.76330 factor:1 | 1 (-1.83595) | -1 | -1 |
| G: -6727.42770 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12993.54472 HOMO: -6.43821 LUMO: 2.10072 factor:1 | 1 (-1.75132) | -1 | -1 |
| G: -6727.42770 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12993.28327 HOMO: -6.42189 LUMO: 2.19596 factor:1 | 1 (-1.48988) | -1 | -1 |
| G: -6727.42770 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12993.34336 HOMO: -6.40556 LUMO: 2.02181 factor:1 | 1 (-1.54996) | -1 | -1 |
| G: -6727.42770 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12993.11285 HOMO: -6.41372 LUMO: 2.26671 factor:1 | 1 (-1.31945) | -1 | -1 |
| G: -6727.42770 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12992.65706 HOMO: -6.60692 LUMO: 2.09800 factor:1 | 1 (-0.86366) | -1 | -1 |
| G: -6727.42770 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12993.11690 HOMO: -6.75931 LUMO: 1.76602 factor:1 | 1 (-1.32351) | -1 | -1 |
| G: -6727.42770 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12993.00585 HOMO: -6.39195 LUMO: 1.84221 factor:1 | 1 (-1.21246) | -1 | -1 |
| G: -6727.42770 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12993.00974 HOMO: -6.74570 LUMO: 2.04085 factor:1 | 1 (-1.21635) | -1 | -1 |
| G: -6727.42770 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12993.59245 HOMO: -6.77019 LUMO: 2.16875 factor:1 | 1 (-1.79905) | -1 | -1 |
| G: -6727.42770 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12993.29840 HOMO: -6.15522 LUMO: 1.81772 factor:1 | 1 (-1.50501) | -1 | -1 |
| G: -6727.42770 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12993.36477 HOMO: -6.48175 LUMO: 2.02453 factor:1 | 1 (-1.57138) | -1 | -1 |
| G: -6727.42770 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12993.29187 HOMO: -6.57427 LUMO: 1.77962 factor:1 | 1 (-1.49848) | -1 | -1 |
| G: -6727.42770 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12992.96313 HOMO: -6.57699 LUMO: 2.42998 factor:1 | 1 (-1.16974) | -1 | -1 |
| G: -6727.42770 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12992.07743 HOMO: -6.35386 LUMO: 2.25310 factor:1 | 1 (-0.28403) | -1 | -1 |
| G: -6727.42770 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12993.25622 HOMO: -6.80013 LUMO: 2.11160 factor:1 | 1 (-1.46283) | -1 | -1 |
| G: -6727.42770 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12993.07021 HOMO: -6.24229 LUMO: 2.05718 factor:1 | 1 (-1.27681) | -1 | -1 |
| G: -6727.42770 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12993.29606 HOMO: -6.42733 LUMO: 1.76874 factor:1 | 1 (-1.50267) | -1 | -1 |
| G: -6727.42770 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12993.26376 HOMO: -6.56883 LUMO: 2.36195 factor:1 | 1 (-1.47037) | -1 | -1 |
| G: -6727.42770 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12993.29799 HOMO: -6.72665 LUMO: 2.28848 factor:1 | 1 (-1.50460) | -1 | -1 |
| G: -6727.42770 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12992.99954 HOMO: -6.39195 LUMO: 1.79051 factor:1 | 1 (-1.20614) | -1 | -1 |
| G: -6727.42770 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12993.00226 HOMO: -6.70761 LUMO: 0.15510 factor:1 | 1 (-1.20887) | -1 | -1 |
| G: -6727.42770 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12992.84193 HOMO: -6.44366 LUMO: -0.16871 factor:1 | 1 (-1.04854) | -1 | -1 |
| G: -6727.42770 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12991.03578 HOMO: -6.68584 LUMO: 1.69527 factor:1 | -1 (0.75762) | -1 | -1 |
| G: -6727.42770 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12992.69330 HOMO: -6.26950 LUMO: 1.61636 factor:1 | 1 (-0.89991) | -1 | -1 |
| G: -6727.42770 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12991.86137 HOMO: -6.47631 LUMO: 1.98915 factor:1 | 1 (-0.06797) | -1 | -1 |
| G: -6727.42770 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12992.75507 HOMO: -6.58243 LUMO: 1.97283 factor:1 | 1 (-0.96168) | -1 | -1 |
| G: -6727.42770 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12993.18063 HOMO: -6.51713 LUMO: 1.97283 factor:1 | 1 (-1.38724) | -1 | -1 |
| G: -6727.42770 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12993.27916 HOMO: -6.65046 LUMO: 1.69255 factor:1 | 1 (-1.48577) | -1 | -1 |
| G: -6727.42770 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12993.12836 HOMO: -6.26406 LUMO: 2.21773 factor:1 | 1 (-1.33496) | -1 | -1 |
| G: -6727.42770 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12991.14900 HOMO: -6.88992 LUMO: 2.28304 factor:1 | -1 (0.64439) | -1 | -1 |
| G: -6727.42770 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12993.09715 HOMO: -6.67767 LUMO: 2.34834 factor:1 | 1 (-1.30375) | -1 | -1 |
| G: -6727.42770 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12993.17005 HOMO: -6.52801 LUMO: 2.10344 factor:1 | 1 (-1.37665) | -1 | -1 |
| G: -6727.42770 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12993.44227 HOMO: -6.52801 LUMO: 2.24222 factor:1 | 1 (-1.64887) | -1 | -1 |
| G: -6727.42770 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12993.27769 HOMO: -6.17154 LUMO: 1.89663 factor:1 | 1 (-1.48430) | -1 | -1 |
| G: -6727.42770 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12993.41508 HOMO: -6.42733 LUMO: 2.15514 factor:1 | 1 (-1.62169) | -1 | -1 |
| G: -6727.42770 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12993.06185 HOMO: -6.36474 LUMO: 2.01364 factor:1 | 1 (-1.26846) | -1 | -1 |
| G: -6727.42770 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12993.03415 HOMO: -6.82189 LUMO: 1.86942 factor:1 | 1 (-1.24076) | -1 | -1 |
| G: -6727.42770 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12993.13391 HOMO: -6.60148 LUMO: 2.00548 factor:1 | 1 (-1.34051) | -1 | -1 |
| G: -6727.42770 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12990.99431 HOMO: -6.67767 LUMO: 2.15786 factor:1 | -1 (0.79909) | -1 | -1 |
| G: -6727.42770 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12992.84332 HOMO: -6.79196 LUMO: 2.06534 factor:1 | 1 (-1.04992) | -1 | -1 |
| G: -6727.42770 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12992.05378 HOMO: -6.70216 LUMO: 1.83405 factor:1 | 1 (-0.26039) | -1 | -1 |
| G: -6727.42770 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12990.96519 HOMO: -6.58788 LUMO: 1.79051 factor:1 | -1 (0.82821) | -1 | -1 |
| G: -6727.42770 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12991.02495 HOMO: -6.34842 LUMO: 1.80139 factor:1 | -1 (0.76845) | -1 | -1 |
| G: -6727.42770 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12993.10591 HOMO: -6.48175 LUMO: 1.95922 factor:1 | 1 (-1.31251) | -1 | -1 |
| G: -6727.42770 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12992.31594 HOMO: -6.71033 LUMO: 2.02997 factor:1 | 1 (-0.52254) | -1 | -1 |
| G: -6727.42770 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12993.09015 HOMO: -6.89264 LUMO: 2.42726 factor:1 | 1 (-1.29676) | -1 | -1 |
| G: -6727.42770 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12993.05407 HOMO: -6.74570 LUMO: 2.20684 factor:1 | 1 (-1.26068) | -1 | -1 |
| G: -6727.42770 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12993.55144 HOMO: -6.30216 LUMO: 2.15242 factor:1 | 1 (-1.75805) | -1 | -1 |
| G: -6727.42770 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12992.24491 HOMO: -6.94979 LUMO: 2.43814 factor:1 | 1 (-0.45152) | -1 | -1 |
| G: -6727.42770 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12992.36192 HOMO: -6.97972 LUMO: 2.11432 factor:1 | 1 (-0.56853) | -1 | -1 |
| G: -6727.42770 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12993.44853 HOMO: -6.17154 LUMO: 1.98099 factor:1 | 1 (-1.65513) | -1 | -1 |
| G: -6727.42770 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12992.65480 HOMO: -6.74026 LUMO: 2.21501 factor:1 | 1 (-0.86140) | -1 | -1 |
| G: -6727.42770 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12992.41920 HOMO: -6.72393 LUMO: 2.19596 factor:1 | 1 (-0.62581) | -1 | -1 |
| G: -6727.42770 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12993.13551 HOMO: -6.11440 LUMO: 2.10072 factor:1 | 1 (-1.34212) | -1 | -1 |
| G: -6727.42770 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12993.06996 HOMO: -6.34297 LUMO: 1.92657 factor:1 | 1 (-1.27657) | -1 | -1 |
| G: -6727.42770 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12993.50573 HOMO: -6.24773 LUMO: 2.00276 factor:1 | 1 (-1.71233) | -1 | -1 |
| G: -6727.42770 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12992.97772 HOMO: -6.75114 LUMO: 1.98643 factor:1 | 1 (-1.18432) | -1 | -1 |
| G: -6727.42770 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12992.87782 HOMO: -6.69128 LUMO: 2.08711 factor:1 | 1 (-1.08443) | -1 | -1 |
| G: -6727.42770 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12993.63122 HOMO: -6.65318 LUMO: 2.15514 factor:1 | 1 (-1.83783) | -1 | -1 |
| G: -6727.42770 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12993.33084 HOMO: -6.67495 LUMO: 1.72248 factor:1 | 1 (-1.53744) | -1 | -1 |
| G: -6727.42770 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12993.17998 HOMO: -6.58243 LUMO: 1.83405 factor:1 | 1 (-1.38658) | -1 | -1 |
| G: -6727.42770 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12993.17105 HOMO: -6.61237 LUMO: 1.69799 factor:1 | 1 (-1.37766) | -1 | -1 |
| G: -6727.42770 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12990.46842 HOMO: -6.57427 LUMO: 2.29936 factor:1 | -1 (1.32498) | -1 | -1 |
| G: -6727.42770 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12991.77124 HOMO: -6.40012 LUMO: 2.35378 factor:1 | -1 (0.02215) | -1 | -1 |
| G: -6727.42770 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12992.74949 HOMO: -6.90081 LUMO: 2.26671 factor:1 | 1 (-0.95610) | -1 | -1 |
| G: -6727.42770 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12991.97919 HOMO: -6.44910 LUMO: 2.25855 factor:1 | 1 (-0.18580) | -1 | -1 |
| G: -6727.42770 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12992.92392 HOMO: -6.61509 LUMO: 2.26943 factor:1 | 1 (-1.13052) | -1 | -1 |
| G: -6727.42770 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12992.77167 HOMO: -6.78924 LUMO: 2.09256 factor:1 | 1 (-0.97828) | -1 | -1 |
| G: -6727.42770 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12992.54832 HOMO: -6.47087 LUMO: 1.97555 factor:1 | 1 (-0.75493) | -1 | -1 |
| G: -6727.42770 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12992.08268 HOMO: -6.75931 LUMO: 1.98643 factor:1 | 1 (-0.28928) | -1 | -1 |
| G: -6727.42770 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12991.77650 HOMO: -6.17971 LUMO: 2.09800 factor:1 | -1 (0.01690) | -1 | -1 |
| G: -6727.42770 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12992.49330 HOMO: -6.83006 LUMO: 1.91840 factor:1 | 1 (-0.69990) | -1 | -1 |
| G: -6727.42770 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12992.24053 HOMO: -6.72938 LUMO: 2.17419 factor:1 | 1 (-0.44714) | -1 | -1 |
| G: -6727.42770 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12993.12762 HOMO: -6.78924 LUMO: 2.42726 factor:1 | 1 (-1.33423) | -1 | -1 |
| G: -6727.42770 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12993.64965 HOMO: -6.41372 LUMO: 1.93745 factor:1 | 1 (-1.85625) | -1 | -1 |
| G: -6727.42770 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12993.01551 HOMO: -6.85455 LUMO: 2.14970 factor:1 | 1 (-1.22212) | -1 | -1 |
| G: -6727.42770 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12990.76614 HOMO: -6.38651 LUMO: 2.18507 factor:1 | -1 (1.02726) | -1 | -1 |
| G: -6727.42770 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12992.87834 HOMO: -6.81373 LUMO: 2.00548 factor:1 | 1 (-1.08495) | -1 | -1 |
| G: -6727.42770 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12993.01826 HOMO: -6.64774 LUMO: 2.41365 factor:1 | 1 (-1.22487) | -1 | -1 |
| G: -6727.42770 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12990.72959 HOMO: -6.70489 LUMO: 2.31569 factor:1 | -1 (1.06380) | -1 | -1 |
| G: -6727.42770 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12992.02241 HOMO: -6.49264 LUMO: 1.78779 factor:1 | 1 (-0.22901) | -1 | -1 |
| G: -6727.42770 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12992.57039 HOMO: -6.81101 LUMO: 1.86670 factor:1 | 1 (-0.77699) | -1 | -1 |
| G: -6727.42770 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12991.61799 HOMO: -6.72121 LUMO: 1.48846 factor:1 | -1 (0.17540) | -1 | -1 |
| G: -6727.42770 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12992.67488 HOMO: -6.35930 LUMO: 1.78507 factor:1 | 1 (-0.88149) | -1 | -1 |
| G: -6727.42770 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12991.78284 HOMO: -6.38651 LUMO: 2.04358 factor:1 | -1 (0.01056) | -1 | -1 |
| G: -6727.42770 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12992.97494 HOMO: -6.42189 LUMO: 1.99187 factor:1 | 1 (-1.18155) | -1 | -1 |
| G: -6727.42770 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12992.06281 HOMO: -6.69400 LUMO: 1.61091 factor:1 | 1 (-0.26942) | -1 | -1 |
| G: -6727.42770 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12990.93988 HOMO: -6.81101 LUMO: 2.17419 factor:1 | -1 (0.85351) | -1 | -1 |
| G: -6727.42770 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12991.76104 HOMO: -6.90897 LUMO: 2.28576 factor:1 | -1 (0.03235) | -1 | -1 |
| G: -6727.42770 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12991.88801 HOMO: -6.75387 LUMO: 2.31297 factor:1 | 1 (-0.09461) | -1 | -1 |
| G: -6727.42770 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12993.23443 HOMO: -7.05863 LUMO: 2.18780 factor:1 | 1 (-1.44103) | -1 | -1 |
| G: -6727.42770 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12992.35153 HOMO: -6.56611 LUMO: 1.99187 factor:1 | 1 (-0.55813) | -1 | -1 |
| G: -6727.42770 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12993.11356 HOMO: -6.59060 LUMO: 1.86398 factor:1 | 1 (-1.32016) | -1 | -1 |
| G: -6727.42770 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12993.20670 HOMO: -6.59060 LUMO: 1.59459 factor:1 | 1 (-1.41330) | -1 | -1 |
| G: -6727.42770 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12993.31106 HOMO: -6.57699 LUMO: 1.48030 factor:1 | 1 (-1.51766) | -1 | -1 |
| G: -6727.42770 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12993.33119 HOMO: -6.99605 LUMO: 2.30208 factor:1 | 1 (-1.53780) | -1 | -1 |
| G: -6727.42770 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12993.19456 HOMO: -6.42189 LUMO: 2.20412 factor:1 | 1 (-1.40117) | -1 | -1 |
| G: -6727.42770 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12993.02313 HOMO: -7.15115 LUMO: 1.83405 factor:1 | 1 (-1.22974) | 1 | 1 |
| G: -6727.42770 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12993.10030 HOMO: -7.08040 LUMO: 2.21773 factor:1 | 1 (-1.30691) | 1 | 1 |
| G: -6727.42770 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12992.79978 HOMO: -6.72121 LUMO: 1.89663 factor:1 | 1 (-1.00639) | -1 | -1 |
| G: -6727.42770 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12993.03954 HOMO: -6.25590 LUMO: 1.85037 factor:1 | 1 (-1.24615) | -1 | -1 |
| G: -6727.42770 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12992.93401 HOMO: -6.70489 LUMO: 1.98915 factor:1 | 1 (-1.14062) | -1 | -1 |
| G: -6727.42770 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12992.31057 HOMO: -6.53617 LUMO: 2.08439 factor:1 | 1 (-0.51718) | -1 | -1 |
| G: -6727.42770 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12992.81848 HOMO: -6.69944 LUMO: 1.98915 factor:1 | 1 (-1.02508) | -1 | -1 |
| G: -6727.42770 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12993.14000 HOMO: -6.79468 LUMO: 1.96466 factor:1 | 1 (-1.34661) | -1 | -1 |
| G: -6727.42770 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12992.60623 HOMO: -6.79468 LUMO: 1.99459 factor:1 | 1 (-0.81283) | -1 | -1 |
| G: -6727.42770 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12991.90210 HOMO: -6.58788 LUMO: 1.98371 factor:1 | 1 (-0.10871) | -1 | -1 |
| G: -6727.42770 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12993.60796 HOMO: -6.58788 LUMO: 2.16603 factor:1 | 1 (-1.81456) | -1 | -1 |
| G: -6727.42770 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12992.70206 HOMO: -6.56883 LUMO: 1.64085 factor:1 | 1 (-0.90867) | -1 | -1 |
| G: -6727.42770 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12993.02501 HOMO: -7.19197 LUMO: 2.66127 factor:1 | 1 (-1.23161) | 1 | 1 |
| G: -6727.42770 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12993.36831 HOMO: -6.48175 LUMO: 2.40004 factor:1 | 1 (-1.57491) | -1 | -1 |
| G: -6727.42770 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12993.01083 HOMO: -6.18515 LUMO: 2.27759 factor:1 | 1 (-1.21744) | -1 | -1 |
| G: -6727.42770 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12993.01415 HOMO: -6.64774 LUMO: 2.13337 factor:1 | 1 (-1.22076) | -1 | -1 |
| G: -6727.42770 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12993.11132 HOMO: -6.39740 LUMO: 1.95106 factor:1 | 1 (-1.31793) | -1 | -1 |
| G: -6727.42770 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12993.13007 HOMO: -6.59332 LUMO: 1.81772 factor:1 | 1 (-1.33668) | -1 | -1 |
| G: -6727.42770 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12993.36570 HOMO: -6.68312 LUMO: 2.41909 factor:1 | 1 (-1.57230) | -1 | -1 |
| G: -6727.42770 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12992.65610 HOMO: -5.87494 LUMO: 2.18235 factor:1 | 1 (-0.86271) | -1 | -1 |
| G: -6727.42770 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12991.70724 HOMO: -6.30488 LUMO: 2.04902 factor:1 | -1 (0.08615) | -1 | -1 |
| G: -6727.42770 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12992.78435 HOMO: -6.65046 LUMO: 2.05446 factor:1 | 1 (-0.99096) | -1 | -1 |
| G: -6727.42770 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12991.81720 HOMO: -6.55794 LUMO: 2.06807 factor:1 | 1 (-0.02381) | -1 | -1 |
| G: -6727.42770 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12993.11312 HOMO: -6.68040 LUMO: 1.99187 factor:1 | 1 (-1.31973) | -1 | -1 |
| G: -6727.42770 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12991.24718 HOMO: -6.60965 LUMO: 2.18780 factor:1 | -1 (0.54621) | -1 | -1 |
| G: -6727.42770 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12993.01821 HOMO: -6.88176 LUMO: 2.10344 factor:1 | 1 (-1.22481) | -1 | -1 |
| G: -6727.42770 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12992.96876 HOMO: -6.63414 LUMO: 1.70615 factor:1 | 1 (-1.17537) | -1 | -1 |
| G: -6727.42770 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12992.69676 HOMO: -7.15115 LUMO: 2.07351 factor:1 | 1 (-0.90336) | 1 | 1 |
| G: -6727.42770 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12993.08792 HOMO: -6.85727 LUMO: 2.27759 factor:1 | 1 (-1.29453) | -1 | -1 |
| G: -6727.42770 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12991.02799 HOMO: -6.91713 LUMO: 2.28848 factor:1 | -1 (0.76540) | -1 | -1 |
| G: -6727.42770 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12992.87445 HOMO: -7.10217 LUMO: 2.14698 factor:1 | 1 (-1.08105) | 1 | 1 |
| G: -6727.42770 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12992.67115 HOMO: -6.78108 LUMO: 2.45447 factor:1 | 1 (-0.87776) | -1 | -1 |
| G: -6727.42770 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12992.87434 HOMO: -6.78380 LUMO: 2.43542 factor:1 | 1 (-1.08095) | -1 | -1 |
| G: -6727.42770 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12992.77603 HOMO: -6.60965 LUMO: 2.33474 factor:1 | 1 (-0.98263) | -1 | -1 |
| G: -6727.42770 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12992.49044 HOMO: -6.72665 LUMO: 2.25855 factor:1 | 1 (-0.69705) | -1 | -1 |
| G: -6727.42770 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12992.94536 HOMO: -6.27495 LUMO: 2.04358 factor:1 | 1 (-1.15197) | -1 | -1 |
| G: -6727.42770 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12993.10311 HOMO: -6.17426 LUMO: 1.45853 factor:1 | 1 (-1.30971) | -1 | -1 |
| G: -6727.42770 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12993.23467 HOMO: -7.21374 LUMO: 2.33474 factor:1 | 1 (-1.44128) | 1 | 1 |
| G: -6727.42770 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12992.62639 HOMO: -6.94707 LUMO: 1.81772 factor:1 | 1 (-0.83299) | -1 | -1 |
| G: -6727.42770 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12991.58721 HOMO: -6.80829 LUMO: 0.17960 factor:1 | -1 (0.20618) | -1 | -1 |
| G: -6727.42770 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12992.68854 HOMO: -7.19469 LUMO: 1.60819 factor:1 | 1 (-0.89515) | 1 | 1 |
| G: -6727.42770 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12991.88932 HOMO: -6.78652 LUMO: 0.53334 factor:1 | 1 (-0.09592) | -1 | -1 |
| G: -6727.42770 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12992.61099 HOMO: -6.70489 LUMO: 0.74559 factor:1 | 1 (-0.81759) | -1 | -1 |
| G: -6727.42770 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12991.88948 HOMO: -6.72393 LUMO: 0.88981 factor:1 | 1 (-0.09608) | -1 | -1 |
| G: -6727.42770 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12993.00833 HOMO: -4.54430 LUMO: -0.90614 factor:1 | 1 (-1.21493) | -1 | -1 |
| G: -6727.42770 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12993.15592 HOMO: -6.83006 LUMO: 0.47348 factor:1 | 1 (-1.36253) | -1 | -1 |
| G: -6727.42770 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12993.22126 HOMO: -7.07496 LUMO: 0.50613 factor:1 | 1 (-1.42786) | -1 | -1 |
| G: -6727.42770 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12993.50766 HOMO: -6.62053 LUMO: 0.74559 factor:1 | 1 (-1.71426) | -1 | -1 |
| G: -6727.42770 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12993.51830 HOMO: -6.79196 LUMO: 1.80139 factor:1 | 1 (-1.72490) | -1 | -1 |
| G: -6727.42770 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12992.71777 HOMO: -6.71033 LUMO: 0.40817 factor:1 | 1 (-0.92437) | -1 | -1 |
| G: -6727.42770 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12992.66895 HOMO: -6.74026 LUMO: 0.95784 factor:1 | 1 (-0.87555) | -1 | -1 |
| G: -6727.42770 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12992.93927 HOMO: -7.34707 LUMO: 0.40001 factor:1 | 1 (-1.14587) | -1 | -1 |
| G: -6727.42770 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12992.96441 HOMO: -6.19875 LUMO: -0.88709 factor:1 | 1 (-1.17101) | -1 | -1 |
| G: -6727.42770 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12993.05720 HOMO: -6.48719 LUMO: -0.14694 factor:1 | 1 (-1.26381) | -1 | -1 |
| G: -6727.42770 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12992.96289 HOMO: -6.73482 LUMO: -0.01633 factor:1 | 1 (-1.16949) | -1 | -1 |
| G: -6727.42770 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12993.13761 HOMO: -7.05591 LUMO: -0.20136 factor:1 | 1 (-1.34422) | -1 | -1 |
| G: -6727.42770 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12993.08324 HOMO: -6.38651 LUMO: -2.07895 factor:1 | 1 (-1.28985) | -1 | -1 |
| G: -6727.42770 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12993.07402 HOMO: -6.85455 LUMO: -1.03403 factor:1 | 1 (-1.28062) | -1 | -1 |
| G: -6727.42770 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12993.14670 HOMO: -6.72121 LUMO: -0.99322 factor:1 | 1 (-1.35330) | -1 | -1 |
| G: -6727.42770 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12992.95418 HOMO: -6.53890 LUMO: -0.10885 factor:1 | 1 (-1.16078) | -1 | -1 |
| G: -6727.42770 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12992.95040 HOMO: -6.68312 LUMO: 0.21225 factor:1 | 1 (-1.15700) | -1 | -1 |
| G: -6727.42770 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12993.12912 HOMO: -6.68040 LUMO: 0.21225 factor:1 | 1 (-1.33573) | -1 | -1 |
| G: -6727.42770 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12993.10234 HOMO: -6.76475 LUMO: -0.64491 factor:1 | 1 (-1.30895) | -1 | -1 |
| G: -6727.42770 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12993.22684 HOMO: -6.48175 LUMO: 0.41633 factor:1 | 1 (-1.43344) | -1 | -1 |
| G: -6727.42770 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12991.83342 HOMO: -6.42733 LUMO: 0.16599 factor:1 | 1 (-0.04003) | -1 | -1 |
| G: -6727.42770 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12992.73692 HOMO: -6.66679 LUMO: 0.77825 factor:1 | 1 (-0.94353) | -1 | -1 |
| G: -6727.42770 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12993.36311 HOMO: -6.75931 LUMO: -0.73471 factor:1 | 1 (-1.56972) | -1 | -1 |
| G: -6727.42770 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12993.15456 HOMO: -6.53617 LUMO: 0.38096 factor:1 | 1 (-1.36117) | -1 | -1 |
| G: -6727.42770 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12991.96494 HOMO: -6.34297 LUMO: 0.35375 factor:1 | 1 (-0.17154) | -1 | -1 |
| G: -6727.42770 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12992.24483 HOMO: -7.11850 LUMO: -0.03265 factor:1 | 1 (-0.45144) | -1 | -1 |
| G: -6727.42770 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12992.74364 HOMO: -5.21914 LUMO: 1.29798 factor:1 | 1 (-0.95025) | -1 | -1 |
| G: -6727.42770 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12993.31473 HOMO: -7.09129 LUMO: -0.66668 factor:1 | 1 (-1.52133) | -1 | -1 |
| G: -6727.42770 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12992.81997 HOMO: -6.96884 LUMO: -0.31021 factor:1 | 1 (-1.02658) | -1 | -1 |
| G: -6727.42770 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12993.18172 HOMO: -6.51713 LUMO: -0.59865 factor:1 | 1 (-1.38832) | -1 | -1 |
| G: -6727.42770 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12991.93666 HOMO: -6.69400 LUMO: -0.07075 factor:1 | 1 (-0.14327) | -1 | -1 |
| G: -6727.42770 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12992.02654 HOMO: -5.28173 LUMO: 1.17281 factor:1 | 1 (-0.23315) | -1 | -1 |
| G: -6727.42770 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12992.69602 HOMO: -6.54434 LUMO: 0.32109 factor:1 | 1 (-0.90263) | -1 | -1 |
| G: -6727.42770 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12992.91317 HOMO: -6.79740 LUMO: -0.24762 factor:1 | 1 (-1.11978) | -1 | -1 |
| G: -6727.42770 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12992.66057 HOMO: -6.91986 LUMO: -0.14694 factor:1 | 1 (-0.86717) | -1 | -1 |
| G: -6727.42770 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12992.14464 HOMO: -6.75114 LUMO: 0.18504 factor:1 | 1 (-0.35124) | -1 | -1 |
| G: -6727.42770 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12993.40747 HOMO: -6.74842 LUMO: 0.69389 factor:1 | 1 (-1.61407) | -1 | -1 |
| G: -6727.42770 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12992.72620 HOMO: -7.01782 LUMO: 0.56600 factor:1 | 1 (-0.93281) | -1 | -1 |
| G: -6727.42770 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12993.27057 HOMO: -6.47359 LUMO: -0.56600 factor:1 | 1 (-1.47717) | -1 | -1 |
| G: -6727.42770 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12992.74313 HOMO: -6.63686 LUMO: -0.55783 factor:1 | 1 (-0.94973) | -1 | -1 |
| G: -6727.42770 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12992.51137 HOMO: -4.13885 LUMO: -2.05446 factor:1 | 1 (-0.71797) | -1 | -1 |
| G: -6727.42770 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12992.96044 HOMO: -6.34570 LUMO: 0.19864 factor:1 | 1 (-1.16704) | -1 | -1 |
| G: -6727.42770 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12992.61692 HOMO: -6.47903 LUMO: 0.24762 factor:1 | 1 (-0.82353) | -1 | -1 |
| G: -6727.42770 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12993.48921 HOMO: -6.15249 LUMO: 0.32109 factor:1 | 1 (-1.69581) | -1 | -1 |
| G: -6727.42770 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12992.50769 HOMO: -6.84366 LUMO: 0.29116 factor:1 | 1 (-0.71430) | -1 | -1 |
| G: -6727.42770 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12990.37307 HOMO: -6.34297 LUMO: 0.19864 factor:1 | -1 (1.42033) | -1 | -1 |
| G: -6727.42770 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12992.87396 HOMO: -6.51168 LUMO: 0.30749 factor:1 | 1 (-1.08056) | -1 | -1 |
| G: -6727.42770 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12992.96670 HOMO: -6.79468 LUMO: -0.16599 factor:1 | 1 (-1.17330) | -1 | -1 |
| G: -6727.42770 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12992.62146 HOMO: -7.24095 LUMO: 0.15238 factor:1 | 1 (-0.82807) | -1 | -1 |
| G: -6727.42770 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12991.69704 HOMO: -7.06952 LUMO: -0.34558 factor:1 | -1 (0.09636) | -1 | -1 |
| G: -6728.10276 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12991.26024 HOMO: -6.88176 LUMO: 0.02177 factor:1 | -1 (1.20821) | -1 | -1 |
| G: -6728.10276 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12991.00976 HOMO: -6.37291 LUMO: -0.69117 factor:1 | -1 (1.45869) | -1 | -1 |
| G: -6728.10276 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12991.13880 HOMO: -6.83278 LUMO: -0.59049 factor:1 | -1 (1.32966) | -1 | -1 |
| G: -6728.10276 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12990.82383 HOMO: -6.57155 LUMO: -0.33470 factor:1 | -1 (1.64463) | -1 | -1 |
| G: -6728.10276 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12990.59914 HOMO: -6.89537 LUMO: -0.58504 factor:1 | -1 (1.86931) | -1 | -1 |
| G: -6728.10276 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12990.85749 HOMO: -6.57155 LUMO: -0.34831 factor:1 | -1 (1.61097) | -1 | -1 |
| G: -6728.10276 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12990.88976 HOMO: -6.64774 LUMO: -0.95784 factor:1 | -1 (1.57870) | -1 | -1 |
| G: -6728.10276 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12990.95806 HOMO: -6.91713 LUMO: -0.69933 factor:1 | -1 (1.51040) | -1 | -1 |
| G: -6728.10276 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12990.85215 HOMO: -6.80557 LUMO: -0.65035 factor:1 | -1 (1.61630) | -1 | -1 |
| G: -6728.10276 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12991.17102 HOMO: -7.26544 LUMO: -0.79729 factor:1 | -1 (1.29744) | -1 | -1 |
| G: -6728.10276 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12990.83561 HOMO: -6.69128 LUMO: -0.16871 factor:1 | -1 (1.63285) | -1 | -1 |
| G: -6728.10276 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12991.02775 HOMO: -6.88448 LUMO: 0.13061 factor:1 | -1 (1.44071) | -1 | -1 |
| G: -6728.10276 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12990.63471 HOMO: -6.50352 LUMO: 0.12245 factor:1 | -1 (1.83375) | -1 | -1 |
| G: -6728.10276 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12990.80219 HOMO: -6.56067 LUMO: 0.17687 factor:1 | -1 (1.66626) | -1 | -1 |
| G: -6728.10276 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12990.98786 HOMO: -6.70216 LUMO: 0.25034 factor:1 | -1 (1.48060) | -1 | -1 |
| G: -6728.10276 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12990.84347 HOMO: -6.51713 LUMO: -0.78369 factor:1 | -1 (1.62498) | -1 | -1 |
| G: -6728.10276 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12993.82026 HOMO: -6.50352 LUMO: 0.12245 factor:1 | 1 (-1.35181) | -1 | -1 |
| G: -6728.10276 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12993.33114 HOMO: -6.22052 LUMO: -0.83811 factor:1 | 1 (-0.86268) | -1 | -1 |
| G: -6728.10276 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12993.38417 HOMO: -6.51168 LUMO: -0.76464 factor:1 | 1 (-0.91572) | -1 | -1 |
| G: -6728.10276 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12993.53280 HOMO: -7.14571 LUMO: -0.80274 factor:1 | 1 (-1.06435) | -1 | -1 |
| G: -6728.10276 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12993.40551 HOMO: -6.66679 LUMO: -0.88709 factor:1 | 1 (-0.93705) | -1 | -1 |
| G: -6728.10276 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12993.41383 HOMO: -6.76203 LUMO: -1.43948 factor:1 | 1 (-0.94538) | -1 | -1 |
| G: -6728.10276 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12993.43702 HOMO: -6.57427 LUMO: -1.62996 factor:1 | 1 (-0.96856) | -1 | -1 |
| G: -6728.10276 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12993.32866 HOMO: -5.05043 LUMO: 1.24900 factor:1 | 1 (-0.86021) | -1 | -1 |
| G: -6728.10276 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12993.79060 HOMO: -6.53345 LUMO: 0.23130 factor:1 | 1 (-1.32215) | -1 | -1 |
| G: -6728.10276 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12993.27301 HOMO: -7.18381 LUMO: -0.22585 factor:1 | 1 (-0.80456) | -1 | -1 |
| G: -6728.10276 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12993.24926 HOMO: -7.00965 LUMO: -1.79595 factor:1 | 1 (-0.78080) | -1 | -1 |
| G: -6728.10276 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12992.94465 HOMO: -6.08174 LUMO: -0.82995 factor:1 | 1 (-0.47620) | -1 | -1 |
| G: -6728.10276 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12992.08826 HOMO: -6.42189 LUMO: -0.84355 factor:1 | -1 (0.38020) | -1 | -1 |
| G: -6728.10276 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12993.43424 HOMO: -6.53890 LUMO: 0.60409 factor:1 | 1 (-0.96579) | -1 | -1 |
| G: -6728.10276 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12993.31723 HOMO: -6.62869 LUMO: 0.43810 factor:1 | 1 (-0.84878) | -1 | -1 |
| G: -6728.10276 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12993.41081 HOMO: -6.68312 LUMO: 0.64491 factor:1 | 1 (-0.94236) | -1 | -1 |
| G: -6728.10276 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12992.00246 HOMO: -6.42189 LUMO: 1.51295 factor:1 | -1 (0.46599) | -1 | -1 |
| G: -6728.10276 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12992.89241 HOMO: -6.17971 LUMO: 1.67622 factor:1 | 1 (-0.42395) | -1 | -1 |
| G: -6728.10276 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12993.66072 HOMO: -6.79196 LUMO: 1.36873 factor:1 | 1 (-1.19227) | -1 | -1 |
| G: -6728.10276 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12993.11024 HOMO: -7.38517 LUMO: 0.56328 factor:1 | 1 (-0.64178) | 1 | 1 |
| G: -6728.10276 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12992.98642 HOMO: -7.56204 LUMO: 0.71566 factor:1 | 1 (-0.51797) | 1 | 1 |
| G: -6728.10276 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12993.20817 HOMO: -6.45726 LUMO: -1.91840 factor:1 | 1 (-0.73971) | -1 | -1 |
| G: -6728.10276 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12992.98593 HOMO: -6.13073 LUMO: -0.97417 factor:1 | 1 (-0.51748) | -1 | -1 |
| G: -6728.10276 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12993.19535 HOMO: -6.50352 LUMO: -0.69661 factor:1 | 1 (-0.72690) | -1 | -1 |
| G: -6728.10276 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12993.06724 HOMO: -6.76747 LUMO: -1.71976 factor:1 | 1 (-0.59879) | -1 | -1 |
| G: -6728.10276 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12993.17954 HOMO: -6.48447 LUMO: -0.89525 factor:1 | 1 (-0.71109) | -1 | -1 |
| G: -6728.10276 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12993.11247 HOMO: -7.11850 LUMO: -0.71566 factor:1 | 1 (-0.64401) | -1 | -1 |
| G: -6728.10276 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12993.62935 HOMO: -6.80285 LUMO: -0.49253 factor:1 | 1 (-1.16089) | -1 | -1 |
| G: -6728.10276 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12993.54472 HOMO: -6.80557 LUMO: -0.88165 factor:1 | 1 (-1.07626) | -1 | -1 |
| G: -6728.10276 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12993.28327 HOMO: -6.94162 LUMO: -0.08980 factor:1 | 1 (-0.81482) | -1 | -1 |
| G: -6728.10276 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12993.34336 HOMO: -6.97972 LUMO: -0.29388 factor:1 | 1 (-0.87490) | -1 | -1 |
| G: -6728.10276 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12993.11285 HOMO: -6.75114 LUMO: 0.04626 factor:1 | 1 (-0.64439) | -1 | -1 |
| G: -6728.10276 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12992.65706 HOMO: -7.15932 LUMO: 0.68845 factor:1 | 1 (-0.18860) | 1 | 1 |
| G: -6728.10276 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12993.11690 HOMO: -7.36612 LUMO: 0.63675 factor:1 | 1 (-0.64845) | 1 | 1 |
| G: -6728.10276 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12993.00585 HOMO: -7.02598 LUMO: -0.66124 factor:1 | 1 (-0.53740) | -1 | -1 |
| G: -6728.10276 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12993.00974 HOMO: -6.89264 LUMO: -0.54967 factor:1 | 1 (-0.54129) | -1 | -1 |
| G: -6728.10276 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12993.59245 HOMO: -6.97700 LUMO: 0.27756 factor:1 | 1 (-1.12399) | -1 | -1 |
| G: -6728.10276 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12993.29840 HOMO: -6.60965 LUMO: 0.08163 factor:1 | 1 (-0.82995) | -1 | -1 |
| G: -6728.10276 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12993.36477 HOMO: -6.70761 LUMO: 0.40001 factor:1 | 1 (-0.89632) | -1 | -1 |
| G: -6728.10276 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12993.29187 HOMO: -6.69128 LUMO: 0.23674 factor:1 | 1 (-0.82342) | -1 | -1 |
| G: -6728.10276 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12992.96313 HOMO: -6.69128 LUMO: -0.69933 factor:1 | 1 (-0.49468) | -1 | -1 |
| G: -6728.10276 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12992.07743 HOMO: -6.18515 LUMO: -0.85988 factor:1 | -1 (0.39103) | -1 | -1 |
| G: -6728.10276 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12993.25622 HOMO: -6.86815 LUMO: -1.90208 factor:1 | 1 (-0.78777) | -1 | -1 |
| G: -6728.10276 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12993.07021 HOMO: -6.37563 LUMO: -1.74697 factor:1 | 1 (-0.60175) | -1 | -1 |
| G: -6728.10276 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12993.29606 HOMO: -6.75659 LUMO: 0.36463 factor:1 | 1 (-0.82761) | -1 | -1 |
| G: -6728.10276 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12993.26376 HOMO: -6.91441 LUMO: -0.88981 factor:1 | 1 (-0.79531) | -1 | -1 |
| G: -6728.10276 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12993.29799 HOMO: -6.71305 LUMO: -0.29933 factor:1 | 1 (-0.82954) | -1 | -1 |
| G: -6728.10276 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12992.99954 HOMO: -6.91441 LUMO: -1.04492 factor:1 | 1 (-0.53108) | -1 | -1 |
| G: -6728.10276 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12993.00226 HOMO: -6.05453 LUMO: -0.83539 factor:1 | 1 (-0.53381) | -1 | -1 |
| G: -6728.10276 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12992.84193 HOMO: -7.35252 LUMO: -0.45715 factor:1 | 1 (-0.37348) | -1 | -1 |
| G: -6728.10276 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12991.03578 HOMO: -6.41644 LUMO: -0.97417 factor:1 | -1 (1.43268) | -1 | -1 |
| G: -6728.10276 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12992.69330 HOMO: -6.78924 LUMO: 0.36735 factor:1 | 1 (-0.22485) | -1 | -1 |
| G: -6728.10276 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12991.86137 HOMO: -6.74298 LUMO: 0.51974 factor:1 | -1 (0.60709) | -1 | -1 |
| G: -6728.10276 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12992.75507 HOMO: -6.48992 LUMO: 1.44765 factor:1 | 1 (-0.28662) | -1 | -1 |
| G: -6728.10276 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12993.18063 HOMO: -6.12528 LUMO: 1.57826 factor:1 | 1 (-0.71218) | -1 | -1 |
| G: -6728.10276 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12993.27916 HOMO: -6.62325 LUMO: 1.57826 factor:1 | 1 (-0.81071) | -1 | -1 |
| G: -6728.10276 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12993.12836 HOMO: -6.19875 LUMO: 1.29798 factor:1 | 1 (-0.65990) | -1 | -1 |
| G: -6728.10276 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12991.14900 HOMO: -6.74570 LUMO: 1.52112 factor:1 | -1 (1.31945) | -1 | -1 |
| G: -6728.10276 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12993.09715 HOMO: -6.84094 LUMO: 1.48574 factor:1 | 1 (-0.62869) | -1 | -1 |
| G: -6728.10276 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12993.17005 HOMO: -6.85183 LUMO: 0.33470 factor:1 | 1 (-0.70159) | -1 | -1 |
| G: -6728.10276 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12993.44227 HOMO: -6.51168 LUMO: 0.48164 factor:1 | 1 (-0.97381) | -1 | -1 |
| G: -6728.10276 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12993.27769 HOMO: -6.25046 LUMO: 0.75648 factor:1 | 1 (-0.80924) | -1 | -1 |
| G: -6728.10276 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12993.41508 HOMO: -6.65591 LUMO: 0.32109 factor:1 | 1 (-0.94663) | -1 | -1 |
| G: -6728.10276 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12993.06185 HOMO: -6.71033 LUMO: 0.40817 factor:1 | 1 (-0.59340) | -1 | -1 |
| G: -6728.10276 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12993.03415 HOMO: -6.75114 LUMO: 0.73471 factor:1 | 1 (-0.56570) | -1 | -1 |
| G: -6728.10276 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12993.13391 HOMO: -6.50624 LUMO: 0.59321 factor:1 | 1 (-0.66545) | -1 | -1 |
| G: -6728.10276 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12990.99431 HOMO: -6.39740 LUMO: 0.83267 factor:1 | -1 (1.47415) | -1 | -1 |
| G: -6728.10276 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12992.84332 HOMO: -6.44094 LUMO: 0.65579 factor:1 | 1 (-0.37486) | -1 | -1 |
| G: -6728.10276 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12992.05378 HOMO: -6.52257 LUMO: 0.05714 factor:1 | -1 (0.41467) | -1 | -1 |
| G: -6728.10276 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12990.96519 HOMO: -7.10217 LUMO: 0.49797 factor:1 | -1 (1.50327) | -1 | -1 |
| G: -6728.10276 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12991.02495 HOMO: -6.83006 LUMO: 0.55783 factor:1 | -1 (1.44351) | -1 | -1 |
| G: -6728.10276 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12993.10591 HOMO: -6.99333 LUMO: -0.79457 factor:1 | 1 (-0.63745) | -1 | -1 |
| G: -6728.10276 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12992.31594 HOMO: -6.64230 LUMO: 0.32382 factor:1 | -1 (0.15252) | -1 | -1 |
| G: -6728.10276 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12993.09015 HOMO: -6.90897 LUMO: 0.30749 factor:1 | 1 (-0.62170) | -1 | -1 |
| G: -6728.10276 HOMO: -7.26544 LUMO: -1.10478 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12993.05407 HOMO: -7.09129 LUMO: 1.33336 factor:1 | 1 (-0.58562) | 1 | 1 |
| G: -6728.10276 HOMO: -7.26544 LUMO: -1.10478 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12993.55144 HOMO: -6.66951 LUMO: 1.34424 factor:1 | 1 (-1.08299) | -1 | -1 |
| G: -6728.10276 HOMO: -7.26544 LUMO: -1.10478 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12992.24491 HOMO: -7.02870 LUMO: 1.48574 factor:1 | -1 (0.22354) | -1 | -1 |
| G: -6728.10276 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12992.36192 HOMO: -7.26544 LUMO: 0.32926 factor:1 | -1 (0.10653) | -1 | -1 |
| G: -6728.10276 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12993.44853 HOMO: -6.56067 LUMO: -0.45987 factor:1 | 1 (-0.98007) | -1 | -1 |
| G: -6728.10276 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12992.65480 HOMO: -6.54434 LUMO: -0.28300 factor:1 | 1 (-0.18634) | -1 | -1 |
| G: -6728.10276 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12992.41920 HOMO: -7.19469 LUMO: 0.54695 factor:1 | -1 (0.04925) | -1 | -1 |
| G: -6728.10276 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12993.13551 HOMO: -6.47359 LUMO: -0.22041 factor:1 | 1 (-0.66706) | -1 | -1 |
| G: -6728.10276 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12993.06996 HOMO: -6.80013 LUMO: 2.08167 factor:1 | 1 (-0.60151) | -1 | -1 |
| G: -6728.10276 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12993.50573 HOMO: -6.23957 LUMO: 1.67894 factor:1 | 1 (-1.03727) | -1 | -1 |
| G: -6728.10276 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12992.97772 HOMO: -6.75114 LUMO: -0.62858 factor:1 | 1 (-0.50926) | -1 | -1 |
| G: -6728.10276 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12992.87782 HOMO: -6.79468 LUMO: -0.64491 factor:1 | 1 (-0.40937) | -1 | -1 |
| G: -6728.10276 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12993.63122 HOMO: -6.84911 LUMO: -0.69661 factor:1 | 1 (-1.16277) | -1 | -1 |
| G: -6728.10276 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12993.33084 HOMO: -7.54028 LUMO: 0.25851 factor:1 | 1 (-0.86238) | -1 | -1 |
| G: -6728.10276 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12993.17998 HOMO: -6.92802 LUMO: -0.71022 factor:1 | 1 (-0.71152) | -1 | -1 |
| G: -6728.10276 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12993.17105 HOMO: -6.72665 LUMO: -0.46804 factor:1 | 1 (-0.70260) | -1 | -1 |
| G: -6728.10276 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12990.46842 HOMO: -6.63686 LUMO: -0.23674 factor:1 | -1 (2.00004) | -1 | -1 |
| G: -6728.10276 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12991.77124 HOMO: -7.21102 LUMO: 0.54423 factor:1 | -1 (0.69721) | -1 | -1 |
| G: -6728.10276 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12992.74949 HOMO: -6.63414 LUMO: -0.25034 factor:1 | 1 (-0.28104) | -1 | -1 |
| G: -6728.10276 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12991.97919 HOMO: -6.70761 LUMO: -0.31837 factor:1 | -1 (0.48926) | -1 | -1 |
| G: -6728.10276 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12992.92392 HOMO: -6.57155 LUMO: 1.76874 factor:1 | 1 (-0.45546) | -1 | -1 |
| G: -6728.10276 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12992.77167 HOMO: -6.84366 LUMO: 2.04358 factor:1 | 1 (-0.30322) | -1 | -1 |
| G: -6728.10276 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12992.54832 HOMO: -6.60420 LUMO: 1.80139 factor:1 | 1 (-0.07987) | -1 | -1 |
| G: -6728.10276 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12992.08268 HOMO: -7.03686 LUMO: 2.21229 factor:1 | -1 (0.38578) | -1 | -1 |
| G: -6728.10276 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12991.77650 HOMO: -6.77564 LUMO: 1.97555 factor:1 | -1 (0.69196) | -1 | -1 |
| G: -6728.10276 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12992.49330 HOMO: -6.40012 LUMO: 2.17691 factor:1 | 1 (-0.02484) | -1 | -1 |
| G: -6728.10276 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12992.24053 HOMO: -6.80013 LUMO: 2.25582 factor:1 | -1 (0.22792) | -1 | -1 |
| G: -6728.10276 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12993.12762 HOMO: -6.74298 LUMO: 2.31569 factor:1 | 1 (-0.65917) | -1 | -1 |
| G: -6728.10276 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12993.64965 HOMO: -6.68856 LUMO: 1.85854 factor:1 | 1 (-1.18119) | -1 | -1 |
| G: -6728.10276 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12993.01551 HOMO: -6.17971 LUMO: 1.52928 factor:1 | 1 (-0.54706) | -1 | -1 |
| G: -6728.10276 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12990.76614 HOMO: -6.54162 LUMO: 1.91840 factor:1 | -1 (1.70232) | -1 | -1 |
| G: -6728.10276 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12992.87834 HOMO: -6.80013 LUMO: -0.55511 factor:1 | 1 (-0.40989) | -1 | -1 |
| G: -6728.10276 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12993.01826 HOMO: -7.46953 LUMO: 0.28572 factor:1 | 1 (-0.54981) | -1 | -1 |
| G: -6728.10276 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12990.72959 HOMO: -6.61781 LUMO: -0.54967 factor:1 | -1 (1.73886) | -1 | -1 |
| G: -6728.10276 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12992.02241 HOMO: -6.56339 LUMO: -0.47892 factor:1 | -1 (0.44605) | -1 | -1 |
| G: -6728.10276 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12992.57039 HOMO: -6.65591 LUMO: -0.25307 factor:1 | 1 (-0.10193) | -1 | -1 |
| G: -6728.10276 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12991.61799 HOMO: -6.62869 LUMO: -0.23402 factor:1 | -1 (0.85046) | -1 | -1 |
| G: -6728.10276 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12992.67488 HOMO: -6.58243 LUMO: -0.19048 factor:1 | 1 (-0.20643) | -1 | -1 |
| G: -6728.10276 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12991.78284 HOMO: -7.27632 LUMO: 0.52790 factor:1 | -1 (0.68562) | -1 | -1 |
| G: -6728.10276 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12992.97494 HOMO: -7.21102 LUMO: 0.57688 factor:1 | 1 (-0.50649) | -1 | -1 |
| G: -6728.10276 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12992.06281 HOMO: -6.72393 LUMO: -0.53879 factor:1 | -1 (0.40564) | -1 | -1 |
| G: -6728.10276 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12990.93988 HOMO: -7.42054 LUMO: -0.99322 factor:1 | -1 (1.52857) | -1 | -1 |
| G: -6728.10276 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12991.76104 HOMO: -6.88992 LUMO: -0.71838 factor:1 | -1 (0.70741) | -1 | -1 |
| G: -6728.10276 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12991.88801 HOMO: -6.88176 LUMO: -0.61226 factor:1 | -1 (0.58045) | -1 | -1 |
| G: -6728.10276 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12993.23443 HOMO: -7.36340 LUMO: -1.04492 factor:1 | 1 (-0.76597) | -1 | -1 |
| G: -6728.10276 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12992.35153 HOMO: -6.65863 LUMO: -0.41906 factor:1 | -1 (0.11693) | -1 | -1 |
| G: -6728.10276 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12993.11356 HOMO: -7.15115 LUMO: -0.66396 factor:1 | 1 (-0.64510) | -1 | -1 |
| G: -6728.10276 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12993.20670 HOMO: -7.10489 LUMO: -0.64491 factor:1 | 1 (-0.73824) | -1 | -1 |
| G: -6728.10276 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12993.31106 HOMO: -7.20285 LUMO: 0.47892 factor:1 | 1 (-0.84260) | -1 | -1 |
| G: -6728.10276 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12993.33119 HOMO: -6.55794 LUMO: -0.28844 factor:1 | 1 (-0.86274) | -1 | -1 |
| G: -6728.10276 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12993.19456 HOMO: -7.19197 LUMO: -0.69661 factor:1 | 1 (-0.72611) | -1 | -1 |
| G: -6728.10276 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12993.02313 HOMO: -6.56883 LUMO: -0.32926 factor:1 | 1 (-0.55468) | -1 | -1 |
| G: -6728.10276 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12993.10030 HOMO: -6.70761 LUMO: 1.95650 factor:1 | 1 (-0.63185) | -1 | -1 |
| G: -6728.10276 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12992.79978 HOMO: -6.60420 LUMO: 1.80684 factor:1 | 1 (-0.33133) | -1 | -1 |
| G: -6728.10276 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12993.03954 HOMO: -6.84094 LUMO: 1.64085 factor:1 | 1 (-0.57109) | -1 | -1 |
| G: -6728.10276 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12992.93401 HOMO: -6.69128 LUMO: 1.90208 factor:1 | 1 (-0.46556) | -1 | -1 |
| G: -6728.10276 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12992.31057 HOMO: -6.75387 LUMO: 1.70343 factor:1 | -1 (0.15788) | -1 | -1 |
| G: -6728.10276 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12992.81848 HOMO: -7.07496 LUMO: 2.10072 factor:1 | 1 (-0.35002) | -1 | -1 |
| G: -6728.10276 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12993.14000 HOMO: -6.99877 LUMO: 2.24494 factor:1 | 1 (-0.67155) | -1 | -1 |
| G: -6728.10276 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12992.60623 HOMO: -6.63414 LUMO: 2.17691 factor:1 | 1 (-0.13777) | -1 | -1 |
| G: -6728.10276 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12991.90210 HOMO: -6.44638 LUMO: 1.78235 factor:1 | -1 (0.56635) | -1 | -1 |
| G: -6728.10276 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12993.60796 HOMO: -6.87632 LUMO: 1.84221 factor:1 | 1 (-1.13950) | -1 | -1 |
| G: -6728.10276 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12992.70206 HOMO: -6.85183 LUMO: 1.68711 factor:1 | 1 (-0.23361) | -1 | -1 |
| G: -6728.10276 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12993.02501 HOMO: -6.96339 LUMO: 2.26671 factor:1 | 1 (-0.55655) | -1 | -1 |
| G: -6728.10276 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12993.36831 HOMO: -6.63141 LUMO: 1.96738 factor:1 | 1 (-0.89985) | -1 | -1 |
| G: -6728.10276 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12993.01083 HOMO: -6.37019 LUMO: 2.23133 factor:1 | 1 (-0.54238) | -1 | -1 |
| G: -6728.10276 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12993.01415 HOMO: -7.11034 LUMO: 2.32385 factor:1 | 1 (-0.54570) | 1 | 1 |
| G: -6728.10276 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12993.11132 HOMO: -6.91986 LUMO: 1.65445 factor:1 | 1 (-0.64287) | -1 | -1 |
| G: -6728.10276 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12993.13007 HOMO: -7.12938 LUMO: 2.28304 factor:1 | 1 (-0.66162) | 1 | 1 |
| G: -6728.10276 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12993.36570 HOMO: -6.54978 LUMO: 1.92112 factor:1 | 1 (-0.89724) | -1 | -1 |
| G: -6728.10276 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12992.65610 HOMO: -6.83006 LUMO: 2.48712 factor:1 | 1 (-0.18765) | -1 | -1 |
| G: -6728.10276 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12991.70724 HOMO: -6.97972 LUMO: 1.96738 factor:1 | -1 (0.76121) | -1 | -1 |
| G: -6728.10276 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12992.78435 HOMO: -6.69944 LUMO: 2.06262 factor:1 | 1 (-0.31590) | -1 | -1 |
| G: -6728.10276 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12991.81720 HOMO: -6.76747 LUMO: 2.10888 factor:1 | -1 (0.65125) | -1 | -1 |
| G: -6728.10276 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12993.11312 HOMO: -6.91169 LUMO: 2.06534 factor:1 | 1 (-0.64466) | -1 | -1 |
| G: -6728.10276 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12991.24718 HOMO: -7.03414 LUMO: 1.93473 factor:1 | -1 (1.22127) | -1 | -1 |
| G: -6728.10276 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12993.01821 HOMO: -7.03142 LUMO: 2.52250 factor:1 | 1 (-0.54975) | -1 | -1 |
| G: -6728.10276 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12992.96876 HOMO: -6.34025 LUMO: 2.61229 factor:1 | 1 (-0.50031) | -1 | -1 |
| G: -6728.10276 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12992.69676 HOMO: -6.98788 LUMO: 2.28304 factor:1 | 1 (-0.22830) | -1 | -1 |
| G: -6728.10276 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12993.08792 HOMO: -6.97700 LUMO: 2.53882 factor:1 | 1 (-0.61947) | -1 | -1 |
| G: -6728.10276 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12991.02799 HOMO: -6.58788 LUMO: 1.94289 factor:1 | -1 (1.44046) | -1 | -1 |
| G: -6728.10276 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12992.87445 HOMO: -6.78652 LUMO: 2.13609 factor:1 | 1 (-0.40599) | -1 | -1 |
| G: -6728.10276 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12992.67115 HOMO: -6.55250 LUMO: 1.82861 factor:1 | 1 (-0.20270) | -1 | -1 |
| G: -6728.10276 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12992.87434 HOMO: -6.45998 LUMO: 1.75786 factor:1 | 1 (-0.40589) | -1 | -1 |
| G: -6728.10276 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12992.77603 HOMO: -6.78924 LUMO: 2.33746 factor:1 | 1 (-0.30757) | -1 | -1 |
| G: -6728.10276 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12992.49044 HOMO: -6.85727 LUMO: 1.76058 factor:1 | 1 (-0.02199) | -1 | -1 |
| G: -6728.10276 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12992.94536 HOMO: -6.70489 LUMO: 1.84493 factor:1 | 1 (-0.47691) | -1 | -1 |
| G: -6728.10276 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12993.10311 HOMO: -6.71305 LUMO: 1.53472 factor:1 | 1 (-0.63465) | -1 | -1 |
| G: -6728.10276 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12993.23467 HOMO: -6.76747 LUMO: 1.48846 factor:1 | 1 (-0.76622) | -1 | -1 |
| G: -6728.10276 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12992.62639 HOMO: -6.69128 LUMO: 1.95922 factor:1 | 1 (-0.15793) | -1 | -1 |
| G: -6728.10276 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12991.58721 HOMO: -6.67495 LUMO: 2.05446 factor:1 | -1 (0.88124) | -1 | -1 |
| G: -6728.10276 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12992.68854 HOMO: -6.63686 LUMO: 2.25310 factor:1 | 1 (-0.22009) | -1 | -1 |
| G: -6728.10276 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12991.88932 HOMO: -6.63958 LUMO: 2.14154 factor:1 | -1 (0.57914) | -1 | -1 |
| G: -6728.10276 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12992.61099 HOMO: -6.62597 LUMO: 2.01908 factor:1 | 1 (-0.14253) | -1 | -1 |
| G: -6728.10276 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12991.88948 HOMO: -7.07768 LUMO: 2.14154 factor:1 | -1 (0.57898) | -1 | -1 |
| G: -6728.10276 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12993.00833 HOMO: -6.19603 LUMO: 2.01092 factor:1 | 1 (-0.53987) | -1 | -1 |
| G: -6728.10276 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12993.15592 HOMO: -6.65046 LUMO: 2.15786 factor:1 | 1 (-0.68747) | -1 | -1 |
| G: -6728.10276 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12993.22126 HOMO: -6.92258 LUMO: 2.31841 factor:1 | 1 (-0.75280) | -1 | -1 |
| G: -6728.10276 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12993.50766 HOMO: -6.90081 LUMO: 2.19324 factor:1 | 1 (-1.03920) | -1 | -1 |
| G: -6728.10276 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12993.51830 HOMO: -6.85455 LUMO: 1.95650 factor:1 | 1 (-1.04984) | -1 | -1 |
| G: -6728.10276 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12992.71777 HOMO: -6.57699 LUMO: 1.76058 factor:1 | 1 (-0.24931) | -1 | -1 |
| G: -6728.10276 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12992.66895 HOMO: -6.90625 LUMO: 1.97555 factor:1 | 1 (-0.20049) | -1 | -1 |
| G: -6728.10276 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12992.93927 HOMO: -6.97428 LUMO: 1.92929 factor:1 | 1 (-0.47081) | -1 | -1 |
| G: -6728.10276 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12992.96441 HOMO: -6.61781 LUMO: -0.41906 factor:1 | 1 (-0.49595) | -1 | -1 |
| G: -6728.10276 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12993.05720 HOMO: -6.62869 LUMO: -0.81906 factor:1 | 1 (-0.58875) | -1 | -1 |
| G: -6728.10276 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12992.96289 HOMO: -7.01237 LUMO: 2.00548 factor:1 | 1 (-0.49443) | -1 | -1 |
| G: -6728.10276 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12993.13761 HOMO: -6.85727 LUMO: 2.17691 factor:1 | 1 (-0.66916) | -1 | -1 |
| G: -6728.10276 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12993.08324 HOMO: -6.71849 LUMO: 1.58914 factor:1 | 1 (-0.61479) | -1 | -1 |
| G: -6728.10276 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12993.07402 HOMO: -7.52395 LUMO: 0.27211 factor:1 | 1 (-0.60556) | -1 | -1 |
| G: -6728.10276 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12993.14670 HOMO: -6.96611 LUMO: -0.72654 factor:1 | 1 (-0.67824) | -1 | -1 |
| G: -6728.10276 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12992.95418 HOMO: -6.89537 LUMO: -0.68028 factor:1 | 1 (-0.48572) | -1 | -1 |
| G: -6728.10276 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12992.95040 HOMO: -6.84911 LUMO: -0.58504 factor:1 | 1 (-0.48194) | -1 | -1 |
| G: -6728.10276 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12993.12912 HOMO: -6.79196 LUMO: -0.55783 factor:1 | 1 (-0.66067) | -1 | -1 |
| G: -6728.10276 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12993.10234 HOMO: -6.67767 LUMO: 1.79323 factor:1 | 1 (-0.63389) | -1 | -1 |
| G: -6728.10276 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12993.22684 HOMO: -6.54434 LUMO: 1.91024 factor:1 | 1 (-0.75838) | -1 | -1 |
| G: -6728.10276 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12991.83342 HOMO: -6.62869 LUMO: 1.69799 factor:1 | -1 (0.63503) | -1 | -1 |
| G: -6728.10276 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12992.73692 HOMO: -6.72393 LUMO: 2.12249 factor:1 | 1 (-0.26847) | -1 | -1 |
| G: -6728.10276 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12993.36311 HOMO: -6.66407 LUMO: 2.05990 factor:1 | 1 (-0.89466) | -1 | -1 |
| G: -6728.10276 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12993.15456 HOMO: -7.00149 LUMO: 1.82044 factor:1 | 1 (-0.68611) | -1 | -1 |
| G: -6728.10276 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12991.96494 HOMO: -7.12122 LUMO: 2.16058 factor:1 | -1 (0.50352) | 1 | 1 |
| G: -6728.10276 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12992.24483 HOMO: -6.63141 LUMO: 2.21229 factor:1 | -1 (0.22362) | -1 | -1 |
| G: -6728.10276 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12992.74364 HOMO: -6.37835 LUMO: 2.32113 factor:1 | 1 (-0.27519) | -1 | -1 |
| G: -6728.10276 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12993.31473 HOMO: -6.99605 LUMO: 2.00548 factor:1 | 1 (-0.84627) | -1 | -1 |
| G: -6728.10276 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12992.81997 HOMO: -6.85999 LUMO: 2.39460 factor:1 | 1 (-0.35152) | -1 | -1 |
| G: -6728.10276 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12993.18172 HOMO: -6.85727 LUMO: 2.48712 factor:1 | 1 (-0.71326) | -1 | -1 |
| G: -6728.10276 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12991.93666 HOMO: -7.04231 LUMO: 2.40277 factor:1 | -1 (0.53179) | -1 | -1 |
| G: -6728.10276 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12992.02654 HOMO: -6.60692 LUMO: 2.26671 factor:1 | -1 (0.44191) | -1 | -1 |
| G: -6728.10276 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12992.69602 HOMO: -6.67495 LUMO: 2.14698 factor:1 | 1 (-0.22757) | -1 | -1 |
| G: -6728.10276 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12992.91317 HOMO: -6.73210 LUMO: 2.06807 factor:1 | 1 (-0.44472) | -1 | -1 |
| G: -6728.10276 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12992.66057 HOMO: -7.20013 LUMO: 2.02181 factor:1 | 1 (-0.19211) | 1 | 1 |
| G: -6728.10276 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12992.14464 HOMO: -7.18653 LUMO: 2.29936 factor:1 | -1 (0.32382) | 1 | 1 |
| G: -6728.10276 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12993.40747 HOMO: -6.92802 LUMO: 2.36195 factor:1 | 1 (-0.93901) | -1 | -1 |
| G: -6728.10276 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12992.72620 HOMO: -6.89537 LUMO: 1.78779 factor:1 | 1 (-0.25775) | -1 | -1 |
| G: -6728.10276 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12993.27057 HOMO: -6.96067 LUMO: 2.31297 factor:1 | 1 (-0.80211) | -1 | -1 |
| G: -6728.10276 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12992.74313 HOMO: -6.91441 LUMO: 2.50345 factor:1 | 1 (-0.27467) | -1 | -1 |
| G: -6728.10276 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12992.51137 HOMO: -7.17292 LUMO: 2.12521 factor:1 | 1 (-0.04291) | 1 | 1 |
| G: -6728.10276 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12992.96044 HOMO: -6.93618 LUMO: 2.35106 factor:1 | 1 (-0.49198) | -1 | -1 |
| G: -6728.10276 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12992.61692 HOMO: -6.75931 LUMO: 1.61908 factor:1 | 1 (-0.14847) | -1 | -1 |
| G: -6728.10276 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12993.48921 HOMO: -6.35930 LUMO: 1.23540 factor:1 | 1 (-1.02075) | -1 | -1 |
| G: -6728.10276 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12992.50769 HOMO: -6.17971 LUMO: 1.84493 factor:1 | 1 (-0.03924) | -1 | -1 |
| G: -6728.10276 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12990.37307 HOMO: -6.72665 LUMO: 2.61229 factor:1 | -1 (2.09539) | -1 | -1 |
| G: -6728.10276 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12992.87396 HOMO: -6.62869 LUMO: 2.28304 factor:1 | 1 (-0.40550) | -1 | -1 |
| G: -6728.10276 HOMO: -8.88180 LUMO: 1.02315 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12992.96670 HOMO: -6.58243 LUMO: 0.28028 factor:1 | 1 (-0.49824) | -1 | -1 |
| G: -6728.10276 HOMO: -8.88180 LUMO: 1.02315 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12992.62146 HOMO: -6.79468 LUMO: 0.14966 factor:1 | 1 (-0.15301) | -1 | -1 |
| G: -6728.10276 HOMO: -8.88180 LUMO: 1.02315 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12991.69704 HOMO: -6.63141 LUMO: 0.31021 factor:1 | -1 (0.77142) | -1 | -1 |
| G: -6727.13594 HOMO: -8.88180 LUMO: 1.02315 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12991.26024 HOMO: -6.81101 LUMO: 0.13878 factor:1 | -1 (0.24139) | -1 | -1 |
| G: -6727.13594 HOMO: -8.88180 LUMO: 1.02315 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12991.00976 HOMO: -6.72665 LUMO: 0.65579 factor:1 | -1 (0.49187) | -1 | -1 |
| G: -6727.13594 HOMO: -8.88180 LUMO: 1.02315 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12991.13880 HOMO: -6.53073 LUMO: 0.91430 factor:1 | -1 (0.36284) | -1 | -1 |
| G: -6727.13594 HOMO: -8.88180 LUMO: 1.02315 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12990.82383 HOMO: -7.19197 LUMO: 1.62996 factor:1 | -1 (0.67781) | 1 | 1 |
| G: -6727.13594 HOMO: -8.88180 LUMO: 1.02315 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12990.59914 HOMO: -6.69400 LUMO: 0.84627 factor:1 | -1 (0.90249) | -1 | -1 |
| G: -6727.13594 HOMO: -8.88180 LUMO: 1.02315 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12990.85749 HOMO: -6.76475 LUMO: 0.51974 factor:1 | -1 (0.64415) | -1 | -1 |
| G: -6727.13594 HOMO: -8.88180 LUMO: 1.02315 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12990.88976 HOMO: -6.67767 LUMO: 0.52246 factor:1 | -1 (0.61188) | -1 | -1 |
| G: -6727.13594 HOMO: -8.88180 LUMO: 1.02315 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12990.95806 HOMO: -6.73210 LUMO: 0.94424 factor:1 | -1 (0.54357) | -1 | -1 |
| G: -6727.13594 HOMO: -8.88180 LUMO: 1.02315 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12990.85215 HOMO: -6.97972 LUMO: 0.60409 factor:1 | -1 (0.64948) | -1 | -1 |
| G: -6727.13594 HOMO: -8.88180 LUMO: 1.02315 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12991.17102 HOMO: -7.38517 LUMO: 0.73743 factor:1 | -1 (0.33062) | -1 | -1 |
| G: -6727.13594 HOMO: -8.88180 LUMO: 1.02315 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12990.83561 HOMO: -6.48992 LUMO: 1.08301 factor:1 | -1 (0.66603) | -1 | -1 |
| G: -6727.13594 HOMO: -8.88180 LUMO: 1.02315 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12991.02775 HOMO: -7.18381 LUMO: 1.61908 factor:1 | -1 (0.47389) | 1 | 1 |
| G: -6727.13594 HOMO: -8.88180 LUMO: 1.02315 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12990.63471 HOMO: -6.74842 LUMO: 0.57960 factor:1 | -1 (0.86693) | -1 | -1 |
| G: -6727.13594 HOMO: -8.88180 LUMO: 1.02315 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12990.80219 HOMO: -6.67495 LUMO: 0.77280 factor:1 | -1 (0.69944) | -1 | -1 |
| G: -6727.13594 HOMO: -8.88180 LUMO: 1.02315 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12990.98786 HOMO: -6.74570 LUMO: 0.77280 factor:1 | -1 (0.51378) | -1 | -1 |
| G: -6727.13594 HOMO: -8.88180 LUMO: 1.02315 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12990.84347 HOMO: -6.73754 LUMO: 0.86804 factor:1 | -1 (0.65816) | -1 | -1 |
| G: -6727.13594 HOMO: -8.88180 LUMO: 1.02315 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12993.82026 HOMO: -6.66135 LUMO: 0.94424 factor:1 | 1 (-2.31863) | -1 | -1 |
| G: -6727.13594 HOMO: -8.88180 LUMO: 1.02315 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12993.33114 HOMO: -6.44638 LUMO: 1.00138 factor:1 | 1 (-1.82950) | -1 | -1 |
| G: -6727.13594 HOMO: -8.88180 LUMO: 1.02315 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12993.38417 HOMO: -6.65591 LUMO: 1.02043 factor:1 | 1 (-1.88254) | -1 | -1 |
| G: -6727.13594 HOMO: -8.88180 LUMO: 1.02315 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12993.53280 HOMO: -7.17564 LUMO: 0.50069 factor:1 | 1 (-2.03117) | -1 | -1 |
| G: -6727.13594 HOMO: -8.88180 LUMO: 1.02315 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12993.40551 HOMO: -6.59332 LUMO: 0.79457 factor:1 | 1 (-1.90387) | -1 | -1 |
| G: -6727.13594 HOMO: -8.88180 LUMO: 1.02315 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12993.41383 HOMO: -6.76747 LUMO: 1.73881 factor:1 | 1 (-1.91220) | -1 | -1 |
| G: -6727.13594 HOMO: -8.88180 LUMO: 1.02315 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12993.43702 HOMO: -7.00421 LUMO: 1.07485 factor:1 | 1 (-1.93538) | -1 | -1 |
| G: -6727.13594 HOMO: -8.88180 LUMO: 1.02315 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12993.32866 HOMO: -6.94979 LUMO: 1.67894 factor:1 | 1 (-1.82703) | -1 | -1 |
| G: -6727.13594 HOMO: -8.88180 LUMO: 1.02315 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12993.79060 HOMO: -6.66135 LUMO: 0.47076 factor:1 | 1 (-2.28897) | -1 | -1 |
| G: -6727.13594 HOMO: -8.88180 LUMO: 1.02315 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12993.27301 HOMO: -6.74298 LUMO: 1.85037 factor:1 | 1 (-1.77138) | -1 | -1 |
| G: -6727.13594 HOMO: -8.88180 LUMO: 1.02315 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12993.24926 HOMO: -6.65318 LUMO: 0.95240 factor:1 | 1 (-1.74762) | -1 | -1 |
| G: -6727.13594 HOMO: -8.88180 LUMO: 1.02315 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12992.94465 HOMO: -6.63958 LUMO: 0.78097 factor:1 | 1 (-1.44302) | -1 | -1 |
| G: -6727.13594 HOMO: -8.88180 LUMO: 1.02315 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12992.08826 HOMO: -6.11712 LUMO: 0.40001 factor:1 | 1 (-0.58662) | -1 | -1 |
| G: -6727.13594 HOMO: -8.88180 LUMO: 1.02315 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12993.43424 HOMO: -7.08312 LUMO: 0.92519 factor:1 | 1 (-1.93261) | -1 | -1 |
| G: -6727.13594 HOMO: -8.88180 LUMO: 1.02315 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12993.31723 HOMO: -6.96067 LUMO: 0.54695 factor:1 | 1 (-1.81560) | -1 | -1 |
| G: -6727.13594 HOMO: -8.88180 LUMO: 1.02315 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12993.41081 HOMO: -6.74026 LUMO: 0.60137 factor:1 | 1 (-1.90918) | -1 | -1 |
| G: -6727.13594 HOMO: -8.88180 LUMO: 1.02315 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12992.00246 HOMO: -6.74298 LUMO: 0.59593 factor:1 | 1 (-0.50083) | -1 | -1 |
| G: -6727.13594 HOMO: -8.88180 LUMO: 1.02315 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12992.89241 HOMO: -6.93074 LUMO: 0.60681 factor:1 | 1 (-1.39077) | -1 | -1 |
| G: -6727.13594 HOMO: -8.88180 LUMO: 1.02315 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12993.66072 HOMO: -6.41644 LUMO: 0.35919 factor:1 | 1 (-2.15909) | -1 | -1 |
| G: -6727.13594 HOMO: -8.88180 LUMO: 1.02315 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12993.11024 HOMO: -6.41917 LUMO: 1.73064 factor:1 | 1 (-1.60860) | -1 | -1 |
| G: -6727.13594 HOMO: -8.88180 LUMO: 1.02315 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12992.98642 HOMO: -4.64226 LUMO: -0.87893 factor:1 | 1 (-1.48479) | -1 | -1 |
| G: -6727.13594 HOMO: -8.88180 LUMO: 1.02315 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12993.20817 HOMO: -6.59604 LUMO: 0.90342 factor:1 | 1 (-1.70653) | -1 | -1 |
| G: -6727.13594 HOMO: -8.88180 LUMO: 1.02315 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12992.98593 HOMO: -6.79468 LUMO: 0.50069 factor:1 | 1 (-1.48430) | -1 | -1 |
| G: -6727.13594 HOMO: -8.88180 LUMO: 1.02315 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12993.19535 HOMO: -7.04503 LUMO: 0.52518 factor:1 | 1 (-1.69372) | -1 | -1 |
| G: -6727.13594 HOMO: -8.88180 LUMO: 1.02315 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12993.06724 HOMO: -6.69400 LUMO: 0.54423 factor:1 | 1 (-1.56561) | -1 | -1 |
| G: -6727.13594 HOMO: -8.88180 LUMO: 1.02315 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12993.17954 HOMO: -6.51713 LUMO: 0.95240 factor:1 | 1 (-1.67791) | -1 | -1 |
| G: -6727.13594 HOMO: -8.88180 LUMO: 1.02315 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12993.11247 HOMO: -6.88176 LUMO: 1.79323 factor:1 | 1 (-1.61083) | -1 | -1 |
| G: -6727.13594 HOMO: -8.88180 LUMO: 1.02315 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12993.62935 HOMO: -6.71849 LUMO: 0.28844 factor:1 | 1 (-2.12771) | -1 | -1 |
| G: -6727.13594 HOMO: -8.88180 LUMO: 1.02315 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12993.54472 HOMO: -6.94979 LUMO: 0.51974 factor:1 | 1 (-2.04309) | -1 | -1 |
| G: -6727.13594 HOMO: -8.88180 LUMO: 1.02315 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12993.28327 HOMO: -6.76203 LUMO: 0.94151 factor:1 | 1 (-1.78164) | -1 | -1 |
| G: -6727.13594 HOMO: -8.88180 LUMO: 1.02315 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12993.34336 HOMO: -6.91169 LUMO: 0.89525 factor:1 | 1 (-1.84172) | -1 | -1 |
| G: -6727.13594 HOMO: -8.88180 LUMO: 1.02315 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12993.11285 HOMO: -6.83006 LUMO: 0.89253 factor:1 | 1 (-1.61121) | -1 | -1 |
| G: -6727.13594 HOMO: -8.88180 LUMO: 1.02315 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12992.65706 HOMO: -7.08857 LUMO: 0.60409 factor:1 | 1 (-1.15542) | -1 | -1 |
| G: -6727.13594 HOMO: -8.88180 LUMO: 1.02315 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12993.11690 HOMO: -6.91713 LUMO: 1.76330 factor:1 | 1 (-1.61527) | -1 | -1 |
| G: -6727.13594 HOMO: -8.88180 LUMO: 1.02315 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12993.00585 HOMO: -6.47359 LUMO: 1.56193 factor:1 | 1 (-1.50422) | -1 | -1 |
| G: -6727.13594 HOMO: -6.91169 LUMO: -0.53879 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12993.00974 HOMO: -7.00149 LUMO: 1.47214 factor:1 | 1 (-1.50811) | -1 | -1 |
| G: -6727.13594 HOMO: -6.91169 LUMO: -0.53879 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12993.59245 HOMO: -7.03686 LUMO: 1.97283 factor:1 | 1 (-2.09081) | -1 | -1 |
| G: -6727.13594 HOMO: -6.91169 LUMO: -0.53879 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12993.29840 HOMO: -7.00965 LUMO: 1.64629 factor:1 | 1 (-1.79677) | -1 | -1 |
| G: -6727.13594 HOMO: -6.91169 LUMO: -0.53879 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12993.36477 HOMO: -7.06952 LUMO: 1.67622 factor:1 | 1 (-1.86314) | 1 | -1 |
| G: -6727.13594 HOMO: -6.91169 LUMO: -0.53879 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12993.29187 HOMO: -6.80557 LUMO: 1.70615 factor:1 | 1 (-1.79024) | -1 | -1 |
| G: -6727.13594 HOMO: -6.91169 LUMO: -0.53879 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12992.96313 HOMO: -6.80829 LUMO: 1.71704 factor:1 | 1 (-1.46150) | -1 | -1 |
| G: -6727.13594 HOMO: -6.91169 LUMO: -0.53879 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12992.07743 HOMO: -7.26544 LUMO: 1.89935 factor:1 | 1 (-0.57579) | 1 | -1 |
| G: -6727.13594 HOMO: -7.29809 LUMO: 2.83543 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12993.25622 HOMO: -7.00149 LUMO: 1.47214 factor:1 | 1 (-1.75459) | -1 | -1 |
| G: -6727.13594 HOMO: -7.29809 LUMO: 2.83543 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12993.07021 HOMO: -7.03686 LUMO: 1.97283 factor:1 | 1 (-1.56857) | -1 | -1 |
| G: -6727.13594 HOMO: -7.29809 LUMO: 2.83543 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12993.29606 HOMO: -7.00965 LUMO: 1.64629 factor:1 | 1 (-1.79443) | -1 | -1 |
| G: -6727.13594 HOMO: -7.29809 LUMO: 2.83543 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12993.26376 HOMO: -7.06952 LUMO: 1.67622 factor:1 | 1 (-1.76213) | -1 | -1 |
| G: -6727.13594 HOMO: -7.29809 LUMO: 2.83543 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12993.29799 HOMO: -6.80557 LUMO: 1.70615 factor:1 | 1 (-1.79636) | -1 | -1 |
| G: -6727.13594 HOMO: -7.29809 LUMO: 2.83543 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12992.99954 HOMO: -6.80829 LUMO: 1.71704 factor:1 | 1 (-1.49791) | -1 | -1 |
| G: -6727.13594 HOMO: -7.29809 LUMO: 2.83543 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12993.00226 HOMO: -7.26544 LUMO: 1.89935 factor:1 | 1 (-1.50063) | -1 | -1 |
| G: -6727.13594 HOMO: -7.85865 LUMO: 2.83543 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12992.84193 HOMO: -7.00149 LUMO: 1.75241 factor:1 | 1 (-1.34030) | -1 | -1 |
| G: -6727.13594 HOMO: -7.85865 LUMO: 2.83543 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12991.03578 HOMO: -6.91169 LUMO: 2.07079 factor:1 | -1 (0.46586) | -1 | -1 |
| G: -6727.13594 HOMO: -7.85865 LUMO: 2.83543 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12992.69330 HOMO: -7.11034 LUMO: 1.76330 factor:1 | 1 (-1.19167) | -1 | -1 |
| G: -6727.13594 HOMO: -7.85865 LUMO: 2.83543 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12991.86137 HOMO: -6.87360 LUMO: 2.02725 factor:1 | 1 (-0.35973) | -1 | -1 |
| G: -6727.13594 HOMO: -7.85865 LUMO: 2.83543 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12992.75507 HOMO: -7.08584 LUMO: 1.82044 factor:1 | 1 (-1.25344) | -1 | -1 |
| G: -6727.13594 HOMO: -7.85865 LUMO: 2.83543 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12993.18063 HOMO: -6.90625 LUMO: 1.68166 factor:1 | 1 (-1.67900) | -1 | -1 |
| G: -6727.13594 HOMO: -7.85865 LUMO: 2.83543 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12993.27916 HOMO: -6.71577 LUMO: 1.93201 factor:1 | 1 (-1.77753) | -1 | -1 |
| G: -6727.13594 HOMO: -7.85865 LUMO: 2.83543 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12993.12836 HOMO: -6.99605 LUMO: 2.08439 factor:1 | 1 (-1.62672) | -1 | -1 |
| G: -6727.13594 HOMO: -7.85865 LUMO: 2.83543 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12991.14900 HOMO: -7.02326 LUMO: 1.97010 factor:1 | -1 (0.35263) | -1 | -1 |
| G: -6727.13594 HOMO: -7.85865 LUMO: 2.83543 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12993.09715 HOMO: -6.99877 LUMO: 2.15514 factor:1 | 1 (-1.59551) | -1 | -1 |
| G: -6727.13594 HOMO: -7.85865 LUMO: 2.83543 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12993.17005 HOMO: -6.75387 LUMO: 1.95106 factor:1 | 1 (-1.66841) | -1 | -1 |
| G: -6727.13594 HOMO: -7.85865 LUMO: 2.83543 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12993.44227 HOMO: -7.10761 LUMO: 2.06262 factor:1 | 1 (-1.94063) | -1 | -1 |
| G: -6727.13594 HOMO: -7.85865 LUMO: 2.83543 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12993.27769 HOMO: -7.03142 LUMO: 1.91568 factor:1 | 1 (-1.77606) | -1 | -1 |
| G: -6727.13594 HOMO: -7.85865 LUMO: 2.83543 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12993.41508 HOMO: -6.98788 LUMO: 1.98371 factor:1 | 1 (-1.91345) | -1 | -1 |
| G: -6727.13594 HOMO: -7.85865 LUMO: 2.83543 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12993.06185 HOMO: -6.94707 LUMO: 1.68438 factor:1 | 1 (-1.56022) | -1 | -1 |
| G: -6727.13594 HOMO: -7.85865 LUMO: 2.83543 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12993.03415 HOMO: -6.88176 LUMO: 2.20684 factor:1 | 1 (-1.53252) | -1 | -1 |
| G: -6727.13594 HOMO: -7.85865 LUMO: 2.83543 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12993.13391 HOMO: -6.73210 LUMO: 2.18780 factor:1 | 1 (-1.63227) | -1 | -1 |
| G: -6727.13594 HOMO: -7.85865 LUMO: 2.83543 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12990.99431 HOMO: -6.83822 LUMO: 2.06807 factor:1 | -1 (0.50733) | -1 | -1 |
| G: -6727.13594 HOMO: -7.85865 LUMO: 2.83543 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12992.84332 HOMO: -6.78924 LUMO: 2.42181 factor:1 | 1 (-1.34168) | -1 | -1 |
| G: -6727.13594 HOMO: -7.85865 LUMO: 2.83543 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12992.05378 HOMO: -6.94707 LUMO: 1.71704 factor:1 | 1 (-0.55215) | -1 | -1 |
| G: -6727.13594 HOMO: -7.85865 LUMO: 2.83543 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12990.96519 HOMO: -6.85183 LUMO: 1.78779 factor:1 | -1 (0.53645) | -1 | -1 |
| G: -6727.13594 HOMO: -7.85865 LUMO: 2.83543 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12991.02495 HOMO: -6.98788 LUMO: 1.69799 factor:1 | -1 (0.47669) | -1 | -1 |
| G: -6727.13594 HOMO: -7.85865 LUMO: 2.83543 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12993.10591 HOMO: -6.79468 LUMO: 2.04358 factor:1 | 1 (-1.60427) | -1 | -1 |
| G: -6727.13594 HOMO: -7.85865 LUMO: 2.83543 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12992.31594 HOMO: -6.90081 LUMO: 1.97283 factor:1 | 1 (-0.81430) | -1 | -1 |
| G: -6727.13594 HOMO: -7.85865 LUMO: 2.83543 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12993.09015 HOMO: -6.79468 LUMO: 2.00820 factor:1 | 1 (-1.58852) | -1 | -1 |
| G: -6727.13594 HOMO: -7.85865 LUMO: 2.83543 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12993.05407 HOMO: -7.06408 LUMO: 2.29936 factor:1 | 1 (-1.55244) | -1 | -1 |
| G: -6727.13594 HOMO: -7.85865 LUMO: 2.83543 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12993.55144 HOMO: -6.78924 LUMO: 2.13337 factor:1 | 1 (-2.04981) | -1 | -1 |
| G: -6727.13594 HOMO: -7.85865 LUMO: 2.83543 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12992.24491 HOMO: -6.79468 LUMO: 2.35106 factor:1 | 1 (-0.74328) | -1 | -1 |
| G: -6727.13594 HOMO: -7.85865 LUMO: 2.83543 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12992.36192 HOMO: -6.82734 LUMO: 2.16603 factor:1 | 1 (-0.86029) | -1 | -1 |
| G: -6727.13594 HOMO: -7.85865 LUMO: 2.83543 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12993.44853 HOMO: -6.79740 LUMO: 2.36739 factor:1 | 1 (-1.94689) | -1 | -1 |
| G: -6727.13594 HOMO: -7.85865 LUMO: 2.83543 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12992.65480 HOMO: -7.14027 LUMO: 2.10888 factor:1 | 1 (-1.15316) | -1 | -1 |
| G: -6727.13594 HOMO: -6.61509 LUMO: -0.23674 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12992.41920 HOMO: -6.96067 LUMO: 1.59731 factor:1 | 1 (-0.91757) | -1 | -1 |
| G: -6727.13594 HOMO: -6.61509 LUMO: -0.23674 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12993.13551 HOMO: -6.91169 LUMO: 1.37145 factor:1 | 1 (-1.63388) | -1 | -1 |
| G: -6727.13594 HOMO: -6.61509 LUMO: -0.23674 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12993.06996 HOMO: -6.94707 LUMO: 1.73064 factor:1 | 1 (-1.56833) | -1 | -1 |
| G: -6727.13594 HOMO: -6.61509 LUMO: -0.23674 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12993.50573 HOMO: -7.02326 LUMO: 1.41227 factor:1 | 1 (-2.00409) | -1 | -1 |
| G: -6727.13594 HOMO: -6.61509 LUMO: -0.23674 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12992.97772 HOMO: -6.72121 LUMO: 1.43132 factor:1 | 1 (-1.47608) | -1 | -1 |
| G: -6727.13594 HOMO: -6.61509 LUMO: -0.23674 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12992.87782 HOMO: -6.51168 LUMO: 1.72520 factor:1 | 1 (-1.37619) | -1 | -1 |
| G: -6727.13594 HOMO: -6.61509 LUMO: -0.23674 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12993.63122 HOMO: -6.98516 LUMO: 1.92929 factor:1 | 1 (-2.12959) | -1 | -1 |
| G: -6727.13594 HOMO: -6.61509 LUMO: -0.23674 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12993.33084 HOMO: -6.92802 LUMO: 2.07895 factor:1 | 1 (-1.82920) | -1 | -1 |
| G: -6727.13594 HOMO: -6.61509 LUMO: -0.23674 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12993.17998 HOMO: -7.02326 LUMO: 1.86398 factor:1 | 1 (-1.67834) | -1 | -1 |
| G: -6727.13594 HOMO: -6.61509 LUMO: -0.23674 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12993.17105 HOMO: -6.82462 LUMO: 1.86670 factor:1 | 1 (-1.66942) | -1 | -1 |
| G: -6727.13594 HOMO: -6.61509 LUMO: -0.23674 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12990.46842 HOMO: -6.83278 LUMO: 1.71160 factor:1 | -1 (1.03322) | -1 | -1 |
| G: -6727.13594 HOMO: -6.61509 LUMO: -0.23674 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12991.77124 HOMO: -6.62869 LUMO: 1.69527 factor:1 | 1 (-0.26961) | -1 | -1 |
| G: -6727.13594 HOMO: -6.61509 LUMO: -0.23674 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12992.74949 HOMO: -6.84094 LUMO: 1.27349 factor:1 | 1 (-1.24786) | -1 | -1 |
| G: -6727.13594 HOMO: -6.61509 LUMO: -0.23674 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12991.97919 HOMO: -7.07768 LUMO: 1.27621 factor:1 | 1 (-0.47756) | 1 | -1 |
| G: -6727.13594 HOMO: -6.61509 LUMO: -0.23674 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12992.92392 HOMO: -7.06135 LUMO: 1.55105 factor:1 | 1 (-1.42228) | 1 | -1 |
| G: -6727.13594 HOMO: -6.61509 LUMO: -0.23674 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12992.77167 HOMO: -6.94162 LUMO: 1.64629 factor:1 | 1 (-1.27004) | -1 | -1 |
| G: -6727.13594 HOMO: -6.61509 LUMO: -0.23674 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12992.54832 HOMO: -7.07224 LUMO: 1.65445 factor:1 | 1 (-1.04669) | 1 | -1 |
| G: -6727.13594 HOMO: -6.61509 LUMO: -0.23674 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12992.08268 HOMO: -6.68584 LUMO: 1.91296 factor:1 | 1 (-0.58104) | -1 | -1 |
| G: -6727.13594 HOMO: -6.61509 LUMO: -0.23674 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12991.77650 HOMO: -7.09129 LUMO: 1.73609 factor:1 | 1 (-0.27486) | 1 | -1 |
| G: -6727.13594 HOMO: -6.61509 LUMO: -0.23674 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12992.49330 HOMO: -7.01237 LUMO: 2.01092 factor:1 | 1 (-0.99166) | -1 | -1 |
| G: -6727.13594 HOMO: -6.61509 LUMO: -0.23674 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12992.24053 HOMO: -6.93618 LUMO: 1.63540 factor:1 | 1 (-0.73890) | -1 | -1 |
| G: -6727.13594 HOMO: -6.61509 LUMO: -0.23674 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12993.12762 HOMO: -6.98516 LUMO: 1.64629 factor:1 | 1 (-1.62599) | -1 | -1 |
| G: -6727.13594 HOMO: -6.61509 LUMO: -0.23674 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12993.64965 HOMO: -6.80285 LUMO: 1.95106 factor:1 | 1 (-2.14801) | -1 | -1 |
| G: -6727.13594 HOMO: -6.61509 LUMO: -0.23674 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12993.01551 HOMO: -6.76747 LUMO: 1.88303 factor:1 | 1 (-1.51388) | -1 | -1 |
| G: -6727.13594 HOMO: -6.61509 LUMO: -0.23674 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12990.76614 HOMO: -6.64230 LUMO: 1.90480 factor:1 | -1 (0.73550) | -1 | -1 |
| G: -6727.13594 HOMO: -6.61509 LUMO: -0.23674 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12992.87834 HOMO: -6.93618 LUMO: 2.19324 factor:1 | 1 (-1.37671) | -1 | -1 |
| G: -6727.13594 HOMO: -6.61509 LUMO: -0.23674 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12993.01826 HOMO: -6.95523 LUMO: 1.80684 factor:1 | 1 (-1.51663) | -1 | -1 |
| G: -6727.13594 HOMO: -6.61509 LUMO: -0.23674 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12990.72959 HOMO: -6.66135 LUMO: 1.72792 factor:1 | -1 (0.77204) | -1 | -1 |
| G: -6727.13594 HOMO: -6.61509 LUMO: -0.23674 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12992.02241 HOMO: -6.36202 LUMO: 1.89391 factor:1 | 1 (-0.52077) | -1 | -1 |
| G: -6727.13594 HOMO: -6.61509 LUMO: -0.23674 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12992.57039 HOMO: -7.03959 LUMO: 2.06262 factor:1 | 1 (-1.06875) | -1 | -1 |
| G: -6727.13594 HOMO: -6.61509 LUMO: -0.23674 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12991.61799 HOMO: -7.08584 LUMO: 2.01092 factor:1 | 1 (-0.11636) | 1 | -1 |
| G: -6727.13594 HOMO: -6.80285 LUMO: -0.55783 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12992.67488 HOMO: -6.96067 LUMO: 1.59731 factor:1 | 1 (-1.17325) | -1 | -1 |
| G: -6727.13594 HOMO: -6.80285 LUMO: -0.55783 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12991.78284 HOMO: -6.91169 LUMO: 1.37145 factor:1 | 1 (-0.28120) | -1 | -1 |
| G: -6727.13594 HOMO: -6.80285 LUMO: -0.55783 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12992.97494 HOMO: -6.94707 LUMO: 1.73064 factor:1 | 1 (-1.47331) | -1 | -1 |
| G: -6727.13594 HOMO: -6.80285 LUMO: -0.55783 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12992.06281 HOMO: -7.02326 LUMO: 1.41227 factor:1 | 1 (-0.56118) | -1 | -1 |
| G: -6727.13594 HOMO: -6.80285 LUMO: -0.55783 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12990.93988 HOMO: -6.72121 LUMO: 1.43132 factor:1 | -1 (0.56175) | -1 | -1 |
| G: -6727.13594 HOMO: -6.80285 LUMO: -0.55783 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12991.76104 HOMO: -6.51168 LUMO: 1.72520 factor:1 | 1 (-0.25941) | -1 | -1 |
| G: -6727.13594 HOMO: -6.80285 LUMO: -0.55783 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12991.88801 HOMO: -6.98516 LUMO: 1.92929 factor:1 | 1 (-0.38637) | -1 | -1 |
| G: -6727.13594 HOMO: -6.80285 LUMO: -0.55783 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12993.23443 HOMO: -6.92802 LUMO: 2.07895 factor:1 | 1 (-1.73279) | -1 | -1 |
| G: -6727.13594 HOMO: -6.80285 LUMO: -0.55783 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12992.35153 HOMO: -7.02326 LUMO: 1.86398 factor:1 | 1 (-0.84989) | -1 | -1 |
| G: -6727.13594 HOMO: -6.80285 LUMO: -0.55783 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12993.11356 HOMO: -6.82462 LUMO: 1.86670 factor:1 | 1 (-1.61192) | -1 | -1 |
| G: -6727.13594 HOMO: -6.80285 LUMO: -0.55783 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12993.20670 HOMO: -6.83278 LUMO: 1.71160 factor:1 | 1 (-1.70507) | -1 | -1 |
| G: -6727.13594 HOMO: -6.80285 LUMO: -0.55783 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12993.31106 HOMO: -6.62869 LUMO: 1.69527 factor:1 | 1 (-1.80942) | -1 | -1 |
| G: -6727.13594 HOMO: -6.80285 LUMO: -0.55783 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12993.33119 HOMO: -6.84094 LUMO: 1.27349 factor:1 | 1 (-1.82956) | -1 | -1 |
| G: -6727.13594 HOMO: -6.80285 LUMO: -0.55783 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12993.19456 HOMO: -7.07768 LUMO: 1.27621 factor:1 | 1 (-1.69293) | 1 | -1 |
| G: -6727.13594 HOMO: -6.80285 LUMO: -0.55783 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12993.02313 HOMO: -7.06135 LUMO: 1.55105 factor:1 | 1 (-1.52150) | 1 | -1 |
| G: -6727.13594 HOMO: -6.80285 LUMO: -0.55783 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12993.10030 HOMO: -6.94162 LUMO: 1.64629 factor:1 | 1 (-1.59867) | -1 | -1 |
| G: -6727.13594 HOMO: -6.80285 LUMO: -0.55783 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12992.79978 HOMO: -7.07224 LUMO: 1.65445 factor:1 | 1 (-1.29815) | 1 | -1 |
| G: -6727.13594 HOMO: -6.80285 LUMO: -0.55783 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12993.03954 HOMO: -6.68584 LUMO: 1.91296 factor:1 | 1 (-1.53791) | -1 | -1 |
| G: -6727.13594 HOMO: -6.80285 LUMO: -0.55783 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12992.93401 HOMO: -7.09129 LUMO: 1.73609 factor:1 | 1 (-1.43238) | 1 | -1 |
| G: -6727.13594 HOMO: -6.80285 LUMO: -0.55783 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12992.31057 HOMO: -7.01237 LUMO: 2.01092 factor:1 | 1 (-0.80894) | -1 | -1 |
| G: -6727.13594 HOMO: -6.80285 LUMO: -0.55783 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12992.81848 HOMO: -6.93618 LUMO: 1.63540 factor:1 | 1 (-1.31684) | -1 | -1 |
| G: -6727.13594 HOMO: -6.80285 LUMO: -0.55783 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12993.14000 HOMO: -6.98516 LUMO: 1.64629 factor:1 | 1 (-1.63837) | -1 | -1 |
| G: -6727.13594 HOMO: -6.80285 LUMO: -0.55783 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12992.60623 HOMO: -6.80285 LUMO: 1.95106 factor:1 | 1 (-1.10459) | -1 | -1 |
| G: -6727.13594 HOMO: -6.80285 LUMO: -0.55783 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12991.90210 HOMO: -6.76747 LUMO: 1.88303 factor:1 | 1 (-0.40047) | -1 | -1 |
| G: -6727.13594 HOMO: -6.80285 LUMO: -0.55783 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12993.60796 HOMO: -6.64230 LUMO: 1.90480 factor:1 | 1 (-2.10632) | -1 | -1 |
| G: -6727.13594 HOMO: -6.80285 LUMO: -0.55783 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12992.70206 HOMO: -6.93618 LUMO: 2.19324 factor:1 | 1 (-1.20043) | -1 | -1 |
| G: -6727.13594 HOMO: -6.80285 LUMO: -0.55783 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12993.02501 HOMO: -6.95523 LUMO: 1.80684 factor:1 | 1 (-1.52338) | -1 | -1 |
| G: -6727.13594 HOMO: -6.80285 LUMO: -0.55783 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12993.36831 HOMO: -6.66135 LUMO: 1.72792 factor:1 | 1 (-1.86667) | -1 | -1 |
| G: -6727.13594 HOMO: -6.80285 LUMO: -0.55783 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12993.01083 HOMO: -6.36202 LUMO: 1.89391 factor:1 | 1 (-1.50920) | -1 | -1 |
| G: -6727.13594 HOMO: -6.80285 LUMO: -0.55783 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12993.01415 HOMO: -7.03959 LUMO: 2.06262 factor:1 | 1 (-1.51252) | -1 | -1 |
| G: -6727.13594 HOMO: -6.80285 LUMO: -0.55783 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12993.11132 HOMO: -7.08584 LUMO: 2.01092 factor:1 | 1 (-1.60969) | 1 | -1 |
| G: -6727.13594 HOMO: -7.16476 LUMO: 2.86264 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12993.13007 HOMO: -6.96067 LUMO: 1.59731 factor:1 | 1 (-1.62844) | -1 | -1 |
| G: -6727.13594 HOMO: -7.16476 LUMO: 2.86264 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12993.36570 HOMO: -6.91169 LUMO: 1.37145 factor:1 | 1 (-1.86406) | -1 | -1 |
| G: -6727.13594 HOMO: -7.16476 LUMO: 2.86264 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12992.65610 HOMO: -6.94707 LUMO: 1.73064 factor:1 | 1 (-1.15447) | -1 | -1 |
| G: -6727.13594 HOMO: -7.16476 LUMO: 2.86264 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12991.70724 HOMO: -7.02326 LUMO: 1.41227 factor:1 | 1 (-0.20561) | -1 | -1 |
| G: -6727.13594 HOMO: -7.16476 LUMO: 2.86264 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12992.78435 HOMO: -6.72121 LUMO: 1.43132 factor:1 | 1 (-1.28272) | -1 | -1 |
| G: -6727.13594 HOMO: -7.16476 LUMO: 2.86264 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12991.81720 HOMO: -6.51168 LUMO: 1.72520 factor:1 | 1 (-0.31557) | -1 | -1 |
| G: -6727.13594 HOMO: -7.16476 LUMO: 2.86264 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12993.11312 HOMO: -6.98516 LUMO: 1.92929 factor:1 | 1 (-1.61149) | -1 | -1 |
| G: -6727.13594 HOMO: -7.16476 LUMO: 2.86264 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12991.24718 HOMO: -6.92802 LUMO: 2.07895 factor:1 | -1 (0.25445) | -1 | -1 |
| G: -6727.13594 HOMO: -7.16476 LUMO: 2.86264 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12993.01821 HOMO: -7.02326 LUMO: 1.86398 factor:1 | 1 (-1.51657) | -1 | -1 |
| G: -6727.13594 HOMO: -7.16476 LUMO: 2.86264 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12992.96876 HOMO: -6.82462 LUMO: 1.86670 factor:1 | 1 (-1.46713) | -1 | -1 |
| G: -6727.13594 HOMO: -7.16476 LUMO: 2.86264 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12992.69676 HOMO: -6.83278 LUMO: 1.71160 factor:1 | 1 (-1.19512) | -1 | -1 |
| G: -6727.13594 HOMO: -7.16476 LUMO: 2.86264 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12993.08792 HOMO: -6.62869 LUMO: 1.69527 factor:1 | 1 (-1.58629) | -1 | -1 |
| G: -6727.13594 HOMO: -7.16476 LUMO: 2.86264 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12991.02799 HOMO: -6.84094 LUMO: 1.27349 factor:1 | -1 (0.47364) | -1 | -1 |
| G: -6727.13594 HOMO: -7.16476 LUMO: 2.86264 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12992.87445 HOMO: -7.07768 LUMO: 1.27621 factor:1 | 1 (-1.37281) | -1 | -1 |
| G: -6727.13594 HOMO: -7.16476 LUMO: 2.86264 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12992.67115 HOMO: -7.06135 LUMO: 1.55105 factor:1 | 1 (-1.16952) | -1 | -1 |
| G: -6727.13594 HOMO: -7.16476 LUMO: 2.86264 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12992.87434 HOMO: -6.94162 LUMO: 1.64629 factor:1 | 1 (-1.37271) | -1 | -1 |
| G: -6727.13594 HOMO: -7.16476 LUMO: 2.86264 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12992.77603 HOMO: -7.07224 LUMO: 1.65445 factor:1 | 1 (-1.27439) | -1 | -1 |
| G: -6727.13594 HOMO: -7.16476 LUMO: 2.86264 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12992.49044 HOMO: -6.68584 LUMO: 1.91296 factor:1 | 1 (-0.98881) | -1 | -1 |
| G: -6727.13594 HOMO: -7.16476 LUMO: 2.86264 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12992.94536 HOMO: -7.09129 LUMO: 1.73609 factor:1 | 1 (-1.44373) | -1 | -1 |
| G: -6727.13594 HOMO: -7.16476 LUMO: 2.86264 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12993.10311 HOMO: -7.01237 LUMO: 2.01092 factor:1 | 1 (-1.60147) | -1 | -1 |
| G: -6727.13594 HOMO: -7.16476 LUMO: 2.86264 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12993.23467 HOMO: -6.93618 LUMO: 1.63540 factor:1 | 1 (-1.73304) | -1 | -1 |
| G: -6727.13594 HOMO: -7.16476 LUMO: 2.86264 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12992.62639 HOMO: -6.98516 LUMO: 1.64629 factor:1 | 1 (-1.12476) | -1 | -1 |
| G: -6727.13594 HOMO: -7.16476 LUMO: 2.86264 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12991.58721 HOMO: -6.80285 LUMO: 1.95106 factor:1 | 1 (-0.08558) | -1 | -1 |
| G: -6727.13594 HOMO: -7.16476 LUMO: 2.86264 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12992.68854 HOMO: -6.76747 LUMO: 1.88303 factor:1 | 1 (-1.18691) | -1 | -1 |
| G: -6727.13594 HOMO: -7.16476 LUMO: 2.86264 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12991.88932 HOMO: -6.64230 LUMO: 1.90480 factor:1 | 1 (-0.38768) | -1 | -1 |
| G: -6727.13594 HOMO: -7.16476 LUMO: 2.86264 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12992.61099 HOMO: -6.93618 LUMO: 2.19324 factor:1 | 1 (-1.10935) | -1 | -1 |
| G: -6727.13594 HOMO: -7.16476 LUMO: 2.86264 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12991.88948 HOMO: -6.95523 LUMO: 1.80684 factor:1 | 1 (-0.38784) | -1 | -1 |
| G: -6727.13594 HOMO: -7.16476 LUMO: 2.86264 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12993.00833 HOMO: -6.66135 LUMO: 1.72792 factor:1 | 1 (-1.50669) | -1 | -1 |
| G: -6727.13594 HOMO: -7.16476 LUMO: 2.86264 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12993.15592 HOMO: -6.36202 LUMO: 1.89391 factor:1 | 1 (-1.65429) | -1 | -1 |
| G: -6727.13594 HOMO: -7.16476 LUMO: 2.86264 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12993.22126 HOMO: -7.03959 LUMO: 2.06262 factor:1 | 1 (-1.71962) | -1 | -1 |
| G: -6727.13594 HOMO: -7.16476 LUMO: 2.86264 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12993.50766 HOMO: -7.08584 LUMO: 2.01092 factor:1 | 1 (-2.00602) | -1 | -1 |
| G: -6727.13594 HOMO: -6.50352 LUMO: 2.10888 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12993.51830 HOMO: -6.96067 LUMO: 1.59731 factor:1 | 1 (-2.01666) | 1 | 1 |
| G: -6727.13594 HOMO: -6.50352 LUMO: 2.10888 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12992.71777 HOMO: -6.91169 LUMO: 1.37145 factor:1 | 1 (-1.21613) | -1 | -1 |
| G: -6727.13594 HOMO: -6.50352 LUMO: 2.10888 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12992.66895 HOMO: -6.94707 LUMO: 1.73064 factor:1 | 1 (-1.16731) | 1 | 1 |
| G: -6727.13594 HOMO: -6.50352 LUMO: 2.10888 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12992.93927 HOMO: -7.02326 LUMO: 1.41227 factor:1 | 1 (-1.43763) | -1 | -1 |
| G: -6727.13594 HOMO: -6.50352 LUMO: 2.10888 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12992.96441 HOMO: -6.72121 LUMO: 1.43132 factor:1 | 1 (-1.46278) | -1 | -1 |
| G: -6727.13594 HOMO: -6.50352 LUMO: 2.10888 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12993.05720 HOMO: -6.51168 LUMO: 1.72520 factor:1 | 1 (-1.55557) | 1 | 1 |
| G: -6727.13594 HOMO: -6.50352 LUMO: 2.10888 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12992.96289 HOMO: -6.98516 LUMO: 1.92929 factor:1 | 1 (-1.46125) | 1 | 1 |
| G: -6727.13594 HOMO: -6.50352 LUMO: 2.10888 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12993.13761 HOMO: -6.92802 LUMO: 2.07895 factor:1 | 1 (-1.63598) | 1 | 1 |
| G: -6727.13594 HOMO: -6.50352 LUMO: 2.10888 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12993.08324 HOMO: -7.02326 LUMO: 1.86398 factor:1 | 1 (-1.58161) | 1 | 1 |
| G: -6727.13594 HOMO: -6.50352 LUMO: 2.10888 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12993.07402 HOMO: -6.82462 LUMO: 1.86670 factor:1 | 1 (-1.57238) | 1 | 1 |
| G: -6727.13594 HOMO: -6.50352 LUMO: 2.10888 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12993.14670 HOMO: -6.83278 LUMO: 1.71160 factor:1 | 1 (-1.64506) | 1 | 1 |
| G: -6727.13594 HOMO: -6.50352 LUMO: 2.10888 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12992.95418 HOMO: -6.62869 LUMO: 1.69527 factor:1 | 1 (-1.45254) | 1 | 1 |
| G: -6727.13594 HOMO: -6.50352 LUMO: 2.10888 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12992.95040 HOMO: -6.84094 LUMO: 1.27349 factor:1 | 1 (-1.44876) | -1 | -1 |
| G: -6727.13594 HOMO: -6.50352 LUMO: 2.10888 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12993.12912 HOMO: -7.07768 LUMO: 1.27621 factor:1 | 1 (-1.62749) | -1 | -1 |
| G: -6727.13594 HOMO: -6.50352 LUMO: 2.10888 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12993.10234 HOMO: -7.06135 LUMO: 1.55105 factor:1 | 1 (-1.60071) | -1 | -1 |
| G: -6727.13594 HOMO: -6.50352 LUMO: 2.10888 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12993.22684 HOMO: -6.94162 LUMO: 1.64629 factor:1 | 1 (-1.72520) | 1 | 1 |
| G: -6727.13594 HOMO: -6.50352 LUMO: 2.10888 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12991.83342 HOMO: -7.07224 LUMO: 1.65445 factor:1 | 1 (-0.33179) | 1 | 1 |
| G: -6727.13594 HOMO: -6.50352 LUMO: 2.10888 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12992.73692 HOMO: -6.68584 LUMO: 1.91296 factor:1 | 1 (-1.23529) | 1 | 1 |
| G: -6727.13594 HOMO: -6.50352 LUMO: 2.10888 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12993.36311 HOMO: -7.09129 LUMO: 1.73609 factor:1 | 1 (-1.86148) | 1 | 1 |
| G: -6727.13594 HOMO: -6.50352 LUMO: 2.10888 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12993.15456 HOMO: -7.01237 LUMO: 2.01092 factor:1 | 1 (-1.65293) | 1 | 1 |
| G: -6727.13594 HOMO: -6.50352 LUMO: 2.10888 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12991.96494 HOMO: -6.93618 LUMO: 1.63540 factor:1 | 1 (-0.46330) | 1 | 1 |
| G: -6727.13594 HOMO: -6.50352 LUMO: 2.10888 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12992.24483 HOMO: -6.98516 LUMO: 1.64629 factor:1 | 1 (-0.74320) | 1 | 1 |
| G: -6727.13594 HOMO: -6.50352 LUMO: 2.10888 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12992.74364 HOMO: -6.80285 LUMO: 1.95106 factor:1 | 1 (-1.24201) | 1 | 1 |
| G: -6727.13594 HOMO: -6.50352 LUMO: 2.10888 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12993.31473 HOMO: -6.76747 LUMO: 1.88303 factor:1 | 1 (-1.81309) | 1 | 1 |
| G: -6727.13594 HOMO: -6.50352 LUMO: 2.10888 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12992.81997 HOMO: -6.64230 LUMO: 1.90480 factor:1 | 1 (-1.31834) | 1 | 1 |
| G: -6727.13594 HOMO: -6.50352 LUMO: 2.10888 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12993.18172 HOMO: -6.93618 LUMO: 2.19324 factor:1 | 1 (-1.68009) | 1 | 1 |
| G: -6727.13594 HOMO: -6.50352 LUMO: 2.10888 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12991.93666 HOMO: -6.95523 LUMO: 1.80684 factor:1 | 1 (-0.43503) | 1 | 1 |
| G: -6727.13594 HOMO: -6.50352 LUMO: 2.10888 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12992.02654 HOMO: -6.66135 LUMO: 1.72792 factor:1 | 1 (-0.52491) | 1 | 1 |
| G: -6727.13594 HOMO: -6.50352 LUMO: 2.10888 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12992.69602 HOMO: -6.36202 LUMO: 1.89391 factor:1 | 1 (-1.19439) | -1 | -1 |
| G: -6727.13594 HOMO: -6.50352 LUMO: 2.10888 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12992.91317 HOMO: -7.03959 LUMO: 2.06262 factor:1 | 1 (-1.41154) | 1 | 1 |
| G: -6727.13594 HOMO: -6.50352 LUMO: 2.10888 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12992.66057 HOMO: -7.08584 LUMO: 2.01092 factor:1 | 1 (-1.15893) | 1 | 1 |
| G: -6727.13594 HOMO: -6.59604 LUMO: 2.33746 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12992.14464 HOMO: -6.96067 LUMO: 1.59731 factor:1 | 1 (-0.64301) | 1 | 1 |
| G: -6727.13594 HOMO: -6.59604 LUMO: 2.33746 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12993.40747 HOMO: -6.91169 LUMO: 1.37145 factor:1 | 1 (-1.90583) | -1 | -1 |
| G: -6727.13594 HOMO: -6.59604 LUMO: 2.33746 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12992.72620 HOMO: -6.94707 LUMO: 1.73064 factor:1 | 1 (-1.22457) | 1 | 1 |
| G: -6727.13594 HOMO: -6.59604 LUMO: 2.33746 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12993.27057 HOMO: -7.02326 LUMO: 1.41227 factor:1 | 1 (-1.76893) | -1 | -1 |
| G: -6727.13594 HOMO: -6.59604 LUMO: 2.33746 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12992.74313 HOMO: -6.72121 LUMO: 1.43132 factor:1 | 1 (-1.24149) | -1 | -1 |
| G: -6727.13594 HOMO: -6.59604 LUMO: 2.33746 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12992.51137 HOMO: -6.51168 LUMO: 1.72520 factor:1 | 1 (-1.00973) | -1 | -1 |
| G: -6727.13594 HOMO: -6.59604 LUMO: 2.33746 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12992.96044 HOMO: -6.98516 LUMO: 1.92929 factor:1 | 1 (-1.45880) | 1 | 1 |
| G: -6727.13594 HOMO: -6.59604 LUMO: 2.33746 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12992.61692 HOMO: -6.92802 LUMO: 2.07895 factor:1 | 1 (-1.11529) | 1 | 1 |
| G: -6727.13594 HOMO: -6.59604 LUMO: 2.33746 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12993.48921 HOMO: -7.02326 LUMO: 1.86398 factor:1 | 1 (-1.98757) | 1 | 1 |
| G: -6727.13594 HOMO: -6.59604 LUMO: 2.33746 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12992.50769 HOMO: -6.82462 LUMO: 1.86670 factor:1 | 1 (-1.00606) | 1 | 1 |
| G: -6727.13594 HOMO: -6.59604 LUMO: 2.33746 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12990.37307 HOMO: -6.83278 LUMO: 1.71160 factor:1 | -1 (1.12857) | 1 | 1 |
| G: -6727.13594 HOMO: -6.59604 LUMO: 2.33746 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12992.87396 HOMO: -6.62869 LUMO: 1.69527 factor:1 | 1 (-1.37232) | 1 | 1 |
| G: -6727.13594 HOMO: -6.59604 LUMO: 2.33746 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12992.96670 HOMO: -6.84094 LUMO: 1.27349 factor:1 | 1 (-1.46506) | -1 | -1 |
| G: -6727.13594 HOMO: -6.59604 LUMO: 2.33746 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12992.62146 HOMO: -7.07768 LUMO: 1.27621 factor:1 | 1 (-1.11983) | -1 | -1 |
| G: -6727.13594 HOMO: -6.59604 LUMO: 2.33746 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12991.69704 HOMO: -7.06135 LUMO: 1.55105 factor:1 | 1 (-0.19540) | -1 | -1 |
| G: -6727.38569 HOMO: -6.59604 LUMO: 2.33746 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12991.26024 HOMO: -6.94162 LUMO: 1.64629 factor:1 | -1 (0.49114) | 1 | 1 |
| G: -6727.38569 HOMO: -6.59604 LUMO: 2.33746 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12991.00976 HOMO: -7.07224 LUMO: 1.65445 factor:1 | -1 (0.74162) | 1 | 1 |
| G: -6727.38569 HOMO: -6.59604 LUMO: 2.33746 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12991.13880 HOMO: -6.68584 LUMO: 1.91296 factor:1 | -1 (0.61258) | 1 | 1 |
| G: -6727.38569 HOMO: -6.59604 LUMO: 2.33746 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12990.82383 HOMO: -7.09129 LUMO: 1.73609 factor:1 | -1 (0.92755) | 1 | 1 |
| G: -6727.38569 HOMO: -6.59604 LUMO: 2.33746 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12990.59914 HOMO: -7.01237 LUMO: 2.01092 factor:1 | -1 (1.15224) | 1 | 1 |
| G: -6727.38569 HOMO: -6.59604 LUMO: 2.33746 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12990.85749 HOMO: -6.93618 LUMO: 1.63540 factor:1 | -1 (0.89389) | 1 | 1 |
| G: -6727.38569 HOMO: -6.59604 LUMO: 2.33746 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12990.88976 HOMO: -6.98516 LUMO: 1.64629 factor:1 | -1 (0.86162) | 1 | 1 |
| G: -6727.38569 HOMO: -6.59604 LUMO: 2.33746 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12990.95806 HOMO: -6.80285 LUMO: 1.95106 factor:1 | -1 (0.79332) | 1 | 1 |
| G: -6727.38569 HOMO: -6.59604 LUMO: 2.33746 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12990.85215 HOMO: -6.76747 LUMO: 1.88303 factor:1 | -1 (0.89923) | 1 | 1 |
| G: -6727.38569 HOMO: -6.59604 LUMO: 2.33746 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12991.17102 HOMO: -6.64230 LUMO: 1.90480 factor:1 | -1 (0.58036) | 1 | 1 |
| G: -6727.38569 HOMO: -6.59604 LUMO: 2.33746 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12990.83561 HOMO: -6.93618 LUMO: 2.19324 factor:1 | -1 (0.91577) | 1 | 1 |
| G: -6727.38569 HOMO: -6.59604 LUMO: 2.33746 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12991.02775 HOMO: -6.95523 LUMO: 1.80684 factor:1 | -1 (0.72363) | 1 | 1 |
| G: -6727.38569 HOMO: -6.59604 LUMO: 2.33746 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12990.63471 HOMO: -6.66135 LUMO: 1.72792 factor:1 | -1 (1.11667) | 1 | 1 |
| G: -6727.38569 HOMO: -6.59604 LUMO: 2.33746 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12990.80219 HOMO: -6.36202 LUMO: 1.89391 factor:1 | -1 (0.94919) | -1 | -1 |
| G: -6727.38569 HOMO: -6.59604 LUMO: 2.33746 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12990.98786 HOMO: -7.03959 LUMO: 2.06262 factor:1 | -1 (0.76352) | 1 | 1 |
| G: -6727.38569 HOMO: -6.59604 LUMO: 2.33746 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12990.84347 HOMO: -7.08584 LUMO: 2.01092 factor:1 | -1 (0.90791) | 1 | 1 |
| G: -6727.38569 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12993.82026 HOMO: -7.06135 LUMO: 0.75376 factor:1 | 1 (-2.06888) | 1 | -1 |
| G: -6727.38569 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12993.33114 HOMO: -5.10213 LUMO: 0.77825 factor:1 | 1 (-1.57976) | -1 | -1 |
| G: -6727.38569 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12993.38417 HOMO: -5.84228 LUMO: 0.50341 factor:1 | 1 (-1.63279) | -1 | -1 |
| G: -6727.38569 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12993.53280 HOMO: -5.39874 LUMO: 0.68028 factor:1 | 1 (-1.78142) | -1 | -1 |
| G: -6727.38569 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12993.40551 HOMO: -5.16744 LUMO: 1.14832 factor:1 | 1 (-1.65413) | -1 | -1 |
| G: -6727.38569 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12993.41383 HOMO: -5.80963 LUMO: 0.35647 factor:1 | 1 (-1.66245) | -1 | -1 |
| G: -6727.38569 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12993.43702 HOMO: -5.02322 LUMO: 1.07213 factor:1 | 1 (-1.68564) | -1 | -1 |
| G: -6727.38569 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12993.32866 HOMO: -5.80963 LUMO: 0.56328 factor:1 | 1 (-1.57728) | -1 | -1 |
| G: -6727.38569 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12993.79060 HOMO: -5.45316 LUMO: 0.78369 factor:1 | 1 (-2.03922) | -1 | -1 |
| G: -6727.38569 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12993.27301 HOMO: -5.25452 LUMO: 0.82178 factor:1 | 1 (-1.52163) | -1 | -1 |
| G: -6727.38569 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12993.24926 HOMO: -5.21370 LUMO: 1.03947 factor:1 | 1 (-1.49788) | -1 | -1 |
| G: -6727.38569 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12992.94465 HOMO: -6.04365 LUMO: 0.31837 factor:1 | 1 (-1.19327) | -1 | -1 |
| G: -6727.38569 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12992.08826 HOMO: -5.86405 LUMO: 0.55511 factor:1 | 1 (-0.33688) | -1 | -1 |
| G: -6727.38569 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12993.43424 HOMO: -5.64908 LUMO: 0.71022 factor:1 | 1 (-1.68286) | -1 | -1 |
| G: -6727.38569 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12993.31723 HOMO: -5.94297 LUMO: 0.68301 factor:1 | 1 (-1.56585) | -1 | -1 |
| G: -6727.38569 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12993.41081 HOMO: -6.01916 LUMO: 0.56328 factor:1 | 1 (-1.65943) | -1 | -1 |
| G: -6727.38569 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12992.00246 HOMO: -6.05181 LUMO: 0.35103 factor:1 | 1 (-0.25108) | -1 | -1 |
| G: -6727.38569 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12992.89241 HOMO: -6.08447 LUMO: 0.48436 factor:1 | 1 (-1.14103) | -1 | -1 |
| G: -6727.38569 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12993.66072 HOMO: -5.86950 LUMO: 0.36735 factor:1 | 1 (-1.90934) | -1 | -1 |
| G: -6727.38569 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12993.11024 HOMO: -5.33615 LUMO: 0.65852 factor:1 | 1 (-1.35885) | -1 | -1 |
| G: -6727.38569 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12992.98642 HOMO: -5.36064 LUMO: 0.86804 factor:1 | 1 (-1.23504) | -1 | -1 |
| G: -6727.38569 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12993.20817 HOMO: -5.74160 LUMO: 0.64491 factor:1 | 1 (-1.45679) | -1 | -1 |
| G: -6727.38569 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12992.98593 HOMO: -5.23003 LUMO: 0.66124 factor:1 | 1 (-1.23455) | -1 | -1 |
| G: -6727.38569 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12993.19535 HOMO: -5.77698 LUMO: 0.84083 factor:1 | 1 (-1.44397) | -1 | -1 |
| G: -6727.38569 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12993.06724 HOMO: -5.60555 LUMO: 0.84355 factor:1 | 1 (-1.31586) | -1 | -1 |
| G: -6727.38569 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12993.17954 HOMO: -7.11578 LUMO: -1.62452 factor:1 | 1 (-1.42816) | -1 | -1 |
| G: -6727.38569 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12993.11247 HOMO: -7.23279 LUMO: -1.63813 factor:1 | 1 (-1.36109) | -1 | -1 |
| G: -6727.38569 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12993.62935 HOMO: -6.68312 LUMO: -0.88709 factor:1 | 1 (-1.87797) | -1 | -1 |
| G: -6727.38569 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12993.54472 HOMO: -6.99333 LUMO: -0.88709 factor:1 | 1 (-1.79334) | -1 | -1 |
| G: -6727.38569 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12993.28327 HOMO: -7.40694 LUMO: 0.11973 factor:1 | 1 (-1.53189) | 1 | 1 |
| G: -6727.38569 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12993.34336 HOMO: -6.74026 LUMO: -0.72927 factor:1 | 1 (-1.59197) | -1 | -1 |
| G: -6727.38569 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12993.11285 HOMO: -6.67223 LUMO: -0.70750 factor:1 | 1 (-1.36147) | -1 | -1 |
| G: -6727.38569 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12992.65706 HOMO: -7.06952 LUMO: -1.40139 factor:1 | 1 (-0.90568) | -1 | -1 |
| G: -6727.38569 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12993.11690 HOMO: -7.21374 LUMO: -1.13199 factor:1 | 1 (-1.36552) | -1 | -1 |
| G: -6727.38569 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12993.00585 HOMO: -6.54706 LUMO: -1.34424 factor:1 | 1 (-1.25447) | -1 | -1 |
| G: -6727.38569 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12993.00974 HOMO: -7.51851 LUMO: -1.05852 factor:1 | 1 (-1.25836) | -1 | -1 |
| G: -6727.38569 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12993.59245 HOMO: -7.07224 LUMO: -1.89391 factor:1 | 1 (-1.84107) | -1 | -1 |
| G: -6727.38569 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12993.29840 HOMO: -6.65863 LUMO: -0.46804 factor:1 | 1 (-1.54702) | -1 | -1 |
| G: -6727.38569 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12993.36477 HOMO: -7.24367 LUMO: 0.29388 factor:1 | 1 (-1.61339) | 1 | 1 |
| G: -6727.38569 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12993.29187 HOMO: -7.02326 LUMO: -0.87893 factor:1 | 1 (-1.54049) | -1 | -1 |
| G: -6727.38569 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12992.96313 HOMO: -6.88176 LUMO: 0.71566 factor:1 | 1 (-1.21175) | -1 | -1 |
| G: -6727.38569 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12992.07743 HOMO: -6.46543 LUMO: 1.01498 factor:1 | 1 (-0.32605) | -1 | -1 |
| G: -6727.38569 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12993.25622 HOMO: -6.30760 LUMO: 0.17687 factor:1 | 1 (-1.50484) | -1 | -1 |
| G: -6727.38569 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12993.07021 HOMO: -6.73210 LUMO: -1.06941 factor:1 | 1 (-1.31883) | -1 | -1 |
| G: -6727.38569 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12993.29606 HOMO: -6.83550 LUMO: -0.75920 factor:1 | 1 (-1.54468) | -1 | -1 |
| G: -6727.38569 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12993.26376 HOMO: -6.94707 LUMO: 0.42178 factor:1 | 1 (-1.51238) | -1 | -1 |
| G: -6727.38569 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12993.29799 HOMO: -6.77019 LUMO: -0.38096 factor:1 | 1 (-1.54661) | -1 | -1 |
| G: -6727.38569 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12992.99954 HOMO: -7.34163 LUMO: 0.35103 factor:1 | 1 (-1.24816) | 1 | 1 |
| G: -6727.38569 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12993.00226 HOMO: -6.87632 LUMO: -0.87349 factor:1 | 1 (-1.25088) | -1 | -1 |
| G: -6727.38569 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12992.84193 HOMO: -7.06952 LUMO: -1.47214 factor:1 | 1 (-1.09055) | -1 | -1 |
| G: -6727.38569 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12991.03578 HOMO: -6.58788 LUMO: -0.37824 factor:1 | -1 (0.71561) | -1 | -1 |
| G: -6727.38569 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12992.69330 HOMO: -6.92802 LUMO: -1.24900 factor:1 | 1 (-0.94192) | -1 | -1 |
| G: -6727.38569 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12991.86137 HOMO: -7.01237 LUMO: -1.31975 factor:1 | 1 (-0.10999) | -1 | -1 |
| G: -6727.38569 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12992.75507 HOMO: -6.74842 LUMO: 0.45987 factor:1 | 1 (-1.00369) | -1 | -1 |
| G: -6727.38569 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12993.18063 HOMO: -6.53890 LUMO: 0.94424 factor:1 | 1 (-1.42925) | -1 | -1 |
| G: -6727.38569 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12993.27916 HOMO: -6.52257 LUMO: -0.66940 factor:1 | 1 (-1.52778) | -1 | -1 |
| G: -6727.38569 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12993.12836 HOMO: -6.56883 LUMO: -1.48302 factor:1 | 1 (-1.37698) | -1 | -1 |
| G: -6727.38569 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12991.14900 HOMO: -7.21646 LUMO: 0.13061 factor:1 | -1 (0.60238) | 1 | 1 |
| G: -6727.38569 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12993.09715 HOMO: -6.62597 LUMO: -0.64763 factor:1 | 1 (-1.34577) | -1 | -1 |
| G: -6727.38569 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12993.17005 HOMO: -7.38789 LUMO: 0.31021 factor:1 | 1 (-1.41867) | 1 | 1 |
| G: -6727.38569 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12993.44227 HOMO: -6.74570 LUMO: -0.70750 factor:1 | 1 (-1.69089) | -1 | -1 |
| G: -6727.38569 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12993.27769 HOMO: -6.95251 LUMO: -1.25989 factor:1 | 1 (-1.52631) | -1 | -1 |
| G: -6727.38569 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12993.41508 HOMO: -7.13483 LUMO: -0.76736 factor:1 | 1 (-1.66370) | -1 | -1 |
| G: -6727.38569 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12993.06185 HOMO: -6.93618 LUMO: -1.24628 factor:1 | 1 (-1.31047) | -1 | -1 |
| G: -6727.38569 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12993.03415 HOMO: -7.03686 LUMO: 0.26395 factor:1 | 1 (-1.28277) | -1 | -1 |
| G: -6727.38569 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12993.13391 HOMO: -6.52257 LUMO: -0.84355 factor:1 | 1 (-1.38253) | -1 | -1 |
| G: -6727.38569 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12990.99431 HOMO: -6.83278 LUMO: -0.49525 factor:1 | -1 (0.75708) | -1 | -1 |
| G: -6727.38569 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12992.84332 HOMO: -7.18381 LUMO: -1.64629 factor:1 | 1 (-1.09194) | -1 | -1 |
| G: -6727.38569 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12992.05378 HOMO: -6.74842 LUMO: -0.81090 factor:1 | 1 (-0.30240) | -1 | -1 |
| G: -6727.38569 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12990.96519 HOMO: -7.09401 LUMO: -0.92519 factor:1 | -1 (0.78619) | -1 | -1 |
| G: -6727.38569 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12991.02495 HOMO: -7.20285 LUMO: -0.81634 factor:1 | -1 (0.72644) | -1 | -1 |
| G: -6727.38569 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12993.10591 HOMO: -6.72665 LUMO: 0.77008 factor:1 | 1 (-1.35453) | -1 | -1 |
| G: -6727.38569 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12992.31594 HOMO: -6.80829 LUMO: 0.86532 factor:1 | 1 (-0.56455) | -1 | -1 |
| G: -6727.38569 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12993.09015 HOMO: -6.20964 LUMO: 0.99866 factor:1 | 1 (-1.33877) | -1 | -1 |
| G: -6727.38569 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12993.05407 HOMO: -6.52801 LUMO: 1.07757 factor:1 | 1 (-1.30269) | -1 | -1 |
| G: -6727.38569 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12993.55144 HOMO: -6.74298 LUMO: -0.67756 factor:1 | 1 (-1.80006) | -1 | -1 |
| G: -6727.38569 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12992.24491 HOMO: -7.43959 LUMO: 0.03265 factor:1 | 1 (-0.49353) | 1 | 1 |
| G: -6727.38569 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12992.36192 HOMO: -6.46815 LUMO: -0.29933 factor:1 | 1 (-0.61054) | -1 | -1 |
| G: -6727.38569 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12993.44853 HOMO: -6.70489 LUMO: -0.97145 factor:1 | 1 (-1.69715) | -1 | -1 |
| G: -6727.38569 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12992.65480 HOMO: -6.30216 LUMO: -1.39322 factor:1 | 1 (-0.90342) | -1 | -1 |
| G: -6727.38569 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12992.41920 HOMO: -7.01782 LUMO: -1.07485 factor:1 | 1 (-0.66782) | -1 | -1 |
| G: -6727.38569 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12993.13551 HOMO: -6.93074 LUMO: 0.25851 factor:1 | 1 (-1.38413) | -1 | -1 |
| G: -6727.38569 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12993.06996 HOMO: -7.07224 LUMO: 0.09524 factor:1 | 1 (-1.31858) | 1 | 1 |
| G: -6727.38569 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12993.50573 HOMO: -6.62325 LUMO: -0.45443 factor:1 | 1 (-1.75435) | -1 | -1 |
| G: -6727.38569 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12992.97772 HOMO: -7.09945 LUMO: -1.20274 factor:1 | 1 (-1.22634) | -1 | -1 |
| G: -6727.38569 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12992.87782 HOMO: -6.56067 LUMO: -1.39322 factor:1 | 1 (-1.12644) | -1 | -1 |
| G: -6727.38569 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12993.63122 HOMO: -6.75387 LUMO: -0.72654 factor:1 | 1 (-1.87984) | -1 | -1 |
| G: -6727.38569 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12993.33084 HOMO: -6.28583 LUMO: -2.35651 factor:1 | 1 (-1.57946) | -1 | -1 |
| G: -6727.38569 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12993.17998 HOMO: -6.55522 LUMO: -1.33608 factor:1 | 1 (-1.42860) | -1 | -1 |
| G: -6727.38569 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12993.17105 HOMO: -7.19741 LUMO: -0.93607 factor:1 | 1 (-1.41967) | -1 | -1 |
| G: -6727.38569 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12990.46842 HOMO: -6.39740 LUMO: -1.14832 factor:1 | -1 (1.28296) | -1 | -1 |
| G: -6727.38569 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12991.77124 HOMO: -7.11850 LUMO: -0.97417 factor:1 | 1 (-0.01986) | -1 | -1 |
| G: -6727.38569 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12992.74949 HOMO: -6.57699 LUMO: -1.14016 factor:1 | 1 (-0.99811) | -1 | -1 |
| G: -6727.38569 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12991.97919 HOMO: -6.57699 LUMO: -1.31975 factor:1 | 1 (-0.22781) | -1 | -1 |
| G: -6727.38569 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12992.92392 HOMO: -6.69128 LUMO: -0.76736 factor:1 | 1 (-1.17254) | -1 | -1 |
| G: -6727.38569 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12992.77167 HOMO: -7.25728 LUMO: 0.29660 factor:1 | 1 (-1.02029) | 1 | 1 |
| G: -6727.38569 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12992.54832 HOMO: -6.37019 LUMO: -0.95240 factor:1 | 1 (-0.79694) | -1 | -1 |
| G: -6727.38569 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12992.08268 HOMO: -6.48447 LUMO: -0.55511 factor:1 | 1 (-0.33130) | -1 | -1 |
| G: -6727.38569 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12991.77650 HOMO: -6.37291 LUMO: -0.78641 factor:1 | 1 (-0.02512) | -1 | -1 |
| G: -6727.38569 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12992.49330 HOMO: -6.65863 LUMO: -0.69933 factor:1 | 1 (-0.74192) | -1 | -1 |
| G: -6727.38569 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12992.24053 HOMO: -6.44638 LUMO: -0.16055 factor:1 | 1 (-0.48915) | -1 | -1 |
| G: -6727.38569 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12993.12762 HOMO: -6.41917 LUMO: -0.20136 factor:1 | 1 (-1.37624) | -1 | -1 |
| G: -6727.38569 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12993.64965 HOMO: -7.33347 LUMO: 0.12789 factor:1 | 1 (-1.89827) | 1 | 1 |
| G: -6727.38569 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12993.01551 HOMO: -6.70489 LUMO: -0.52518 factor:1 | 1 (-1.26413) | -1 | -1 |
| G: -6727.38569 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12990.76614 HOMO: -7.25183 LUMO: 0.32109 factor:1 | -1 (0.98524) | 1 | 1 |
| G: -6727.38569 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12992.87834 HOMO: -7.29265 LUMO: 0.28028 factor:1 | 1 (-1.12696) | 1 | 1 |
| G: -6727.38569 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12993.01826 HOMO: -6.57155 LUMO: -0.51702 factor:1 | 1 (-1.26688) | -1 | -1 |
| G: -6727.38569 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12990.72959 HOMO: -7.08040 LUMO: 0.39729 factor:1 | -1 (1.02179) | 1 | 1 |
| G: -6727.38569 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12992.02241 HOMO: -6.24501 LUMO: -0.44627 factor:1 | 1 (-0.27103) | -1 | -1 |
| G: -6727.38569 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12992.57039 HOMO: -6.73754 LUMO: -0.45443 factor:1 | 1 (-0.81901) | -1 | -1 |
| G: -6727.38569 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12991.61799 HOMO: -6.24501 LUMO: 0.38096 factor:1 | -1 (0.13339) | -1 | -1 |
| G: -6727.38569 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12992.67488 HOMO: -6.86815 LUMO: -0.91974 factor:1 | 1 (-0.92350) | -1 | -1 |
| G: -6727.38569 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12991.78284 HOMO: -7.40150 LUMO: 0.36191 factor:1 | 1 (-0.03146) | 1 | 1 |
| G: -6727.38569 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12992.97494 HOMO: -6.44094 LUMO: -0.64219 factor:1 | 1 (-1.22356) | -1 | -1 |
| G: -6727.38569 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12992.06281 HOMO: -6.69944 LUMO: -0.80001 factor:1 | 1 (-0.31143) | -1 | -1 |
| G: -6727.38569 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12990.93988 HOMO: -6.61509 LUMO: -0.70750 factor:1 | -1 (0.81150) | -1 | -1 |
| G: -6727.38569 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12991.76104 HOMO: -7.52123 LUMO: 0.06803 factor:1 | 1 (-0.00966) | 1 | 1 |
| G: -6727.38569 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12991.88801 HOMO: -7.34163 LUMO: 0.30477 factor:1 | 1 (-0.13663) | 1 | 1 |
| G: -6727.38569 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12993.23443 HOMO: -6.68584 LUMO: -0.78641 factor:1 | 1 (-1.48305) | -1 | -1 |
| G: -6727.38569 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12992.35153 HOMO: -6.53890 LUMO: -0.50885 factor:1 | 1 (-0.60015) | -1 | -1 |
| G: -6727.38569 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12993.11356 HOMO: -6.75659 LUMO: -0.68845 factor:1 | 1 (-1.36217) | -1 | -1 |
| G: -6727.38569 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12993.20670 HOMO: -7.08857 LUMO: 0.43266 factor:1 | 1 (-1.45532) | 1 | 1 |
| G: -6727.38569 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12993.31106 HOMO: -6.28583 LUMO: -0.46804 factor:1 | 1 (-1.55968) | -1 | -1 |
| G: -6727.38569 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12993.33119 HOMO: -6.50080 LUMO: -0.24762 factor:1 | 1 (-1.57981) | -1 | -1 |
| G: -6727.38569 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12993.19456 HOMO: -6.45454 LUMO: -0.58504 factor:1 | 1 (-1.44318) | -1 | -1 |
| G: -6727.38569 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12993.02313 HOMO: -7.20558 LUMO: 0.20953 factor:1 | 1 (-1.27175) | 1 | 1 |
| G: -6727.38569 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12993.10030 HOMO: -6.35930 LUMO: -0.20681 factor:1 | 1 (-1.34892) | -1 | -1 |
| G: -6727.38569 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12992.79978 HOMO: -6.36202 LUMO: -0.14422 factor:1 | 1 (-1.04840) | -1 | -1 |
| G: -6727.38569 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12993.03954 HOMO: -6.20692 LUMO: 1.97827 factor:1 | 1 (-1.28816) | -1 | -1 |
| G: -6727.38569 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12992.93401 HOMO: -6.48719 LUMO: 1.74153 factor:1 | 1 (-1.18263) | -1 | -1 |
| G: -6727.38569 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12992.31057 HOMO: -6.84638 LUMO: 1.88575 factor:1 | 1 (-0.55919) | -1 | -1 |
| G: -6727.38569 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12992.81848 HOMO: -5.90759 LUMO: 2.00820 factor:1 | 1 (-1.06709) | -1 | -1 |
| G: -6727.38569 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12993.14000 HOMO: -6.56339 LUMO: 1.99732 factor:1 | 1 (-1.38862) | -1 | -1 |
| G: -6727.38569 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12992.60623 HOMO: -6.20692 LUMO: 1.75241 factor:1 | 1 (-0.85485) | -1 | -1 |
| G: -6727.38569 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12991.90210 HOMO: -6.16882 LUMO: 1.94017 factor:1 | 1 (-0.15072) | -1 | -1 |
| G: -6727.38569 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12993.60796 HOMO: -6.80829 LUMO: 1.78507 factor:1 | 1 (-1.85658) | -1 | -1 |
| G: -6727.38569 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12992.70206 HOMO: -6.58243 LUMO: 1.78235 factor:1 | 1 (-0.95068) | -1 | -1 |
| G: -6727.38569 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12993.02501 HOMO: -5.85045 LUMO: 1.82316 factor:1 | 1 (-1.27363) | -1 | -1 |
| G: -6727.38569 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12993.36831 HOMO: -5.93752 LUMO: 1.56465 factor:1 | 1 (-1.61693) | -1 | -1 |
| G: -6727.38569 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12993.01083 HOMO: -6.59604 LUMO: -0.53334 factor:1 | 1 (-1.25945) | -1 | -1 |
| G: -6727.38569 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12993.01415 HOMO: -7.06135 LUMO: 0.29660 factor:1 | 1 (-1.26277) | 1 | 1 |
| G: -6727.38569 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12993.11132 HOMO: -6.50352 LUMO: 1.61908 factor:1 | 1 (-1.35994) | -1 | -1 |
| G: -6727.38569 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12993.13007 HOMO: -6.68040 LUMO: -0.60681 factor:1 | 1 (-1.37869) | -1 | -1 |
| G: -6727.38569 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12993.36570 HOMO: -6.93618 LUMO: -1.09662 factor:1 | 1 (-1.61432) | -1 | -1 |
| G: -6727.38569 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12992.65610 HOMO: -6.72121 LUMO: -1.14016 factor:1 | 1 (-0.90472) | -1 | -1 |
| G: -6727.38569 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12991.70724 HOMO: -7.12394 LUMO: -1.24900 factor:1 | -1 (0.04414) | -1 | -1 |
| G: -6727.38569 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12992.78435 HOMO: -6.71305 LUMO: -0.71566 factor:1 | 1 (-1.03297) | -1 | -1 |
| G: -6727.38569 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12991.81720 HOMO: -7.09401 LUMO: -0.86532 factor:1 | 1 (-0.06582) | -1 | -1 |
| G: -6727.38569 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12993.11312 HOMO: -7.08584 LUMO: -0.92519 factor:1 | 1 (-1.36174) | -1 | -1 |
| G: -6727.38569 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12991.24718 HOMO: -7.05591 LUMO: 0.11973 factor:1 | -1 (0.50420) | -1 | -1 |
| G: -6727.38569 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12993.01821 HOMO: -7.14843 LUMO: -1.58370 factor:1 | 1 (-1.26683) | -1 | -1 |
| G: -6727.38569 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12992.96876 HOMO: -7.36884 LUMO: -1.97010 factor:1 | 1 (-1.21738) | -1 | -1 |
| G: -6727.38569 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12992.69676 HOMO: -6.81373 LUMO: -1.72248 factor:1 | 1 (-0.94538) | -1 | -1 |
| G: -6727.38569 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12993.08792 HOMO: -6.87360 LUMO: -1.03947 factor:1 | 1 (-1.33654) | -1 | -1 |
| G: -6727.38569 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12991.02799 HOMO: -7.02870 LUMO: -0.87349 factor:1 | -1 (0.72339) | -1 | -1 |
| G: -6727.38569 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12992.87445 HOMO: -7.16476 LUMO: -1.18097 factor:1 | 1 (-1.12307) | -1 | -1 |
| G: -6727.38569 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12992.67115 HOMO: -7.51851 LUMO: 0.07891 factor:1 | 1 (-0.91977) | 1 | 1 |
| G: -6727.38569 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12992.87434 HOMO: -7.04231 LUMO: -0.83539 factor:1 | 1 (-1.12296) | -1 | -1 |
| G: -6727.38569 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12992.77603 HOMO: -6.83278 LUMO: -0.60137 factor:1 | 1 (-1.02464) | -1 | -1 |
| G: -6727.38569 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12992.49044 HOMO: -6.89809 LUMO: -1.19186 factor:1 | 1 (-0.73906) | -1 | -1 |
| G: -6727.38569 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12992.94536 HOMO: -7.16476 LUMO: -0.79185 factor:1 | 1 (-1.19398) | -1 | -1 |
| G: -6727.38569 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12993.10311 HOMO: -6.97156 LUMO: -1.25444 factor:1 | 1 (-1.35173) | -1 | -1 |
| G: -6727.38569 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12993.23467 HOMO: -6.84366 LUMO: -0.88437 factor:1 | 1 (-1.48329) | -1 | -1 |
| G: -6727.38569 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12992.62639 HOMO: -6.91986 LUMO: -1.12655 factor:1 | 1 (-0.87501) | -1 | -1 |
| G: -6727.38569 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12991.58721 HOMO: -6.49536 LUMO: -0.29660 factor:1 | -1 (0.16417) | -1 | -1 |
| G: -6727.38569 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12992.68854 HOMO: -6.74842 LUMO: 0.42450 factor:1 | 1 (-0.93716) | -1 | -1 |
| G: -6727.38569 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12991.88932 HOMO: -7.34435 LUMO: 0.32109 factor:1 | 1 (-0.13793) | 1 | 1 |
| G: -6727.38569 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12992.61099 HOMO: -7.16476 LUMO: 0.28572 factor:1 | 1 (-0.85961) | 1 | 1 |
| G: -6727.38569 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12991.88948 HOMO: -6.74298 LUMO: -0.43538 factor:1 | 1 (-0.13810) | -1 | -1 |
| G: -6727.38569 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12993.00833 HOMO: -7.19469 LUMO: -1.61091 factor:1 | 1 (-1.25695) | -1 | -1 |
| G: -6727.38569 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12993.15592 HOMO: -7.35252 LUMO: -1.78235 factor:1 | 1 (-1.40454) | -1 | -1 |
| G: -6727.38569 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12993.22126 HOMO: -7.25456 LUMO: -1.66806 factor:1 | 1 (-1.46988) | -1 | -1 |
| G: -6727.38569 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12993.50766 HOMO: -7.54844 LUMO: -1.07213 factor:1 | 1 (-1.75628) | -1 | -1 |
| G: -6727.38569 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12993.51830 HOMO: -7.21918 LUMO: -1.55377 factor:1 | 1 (-1.76692) | -1 | -1 |
| G: -6727.38569 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12992.71777 HOMO: -7.01782 LUMO: -1.60547 factor:1 | 1 (-0.96639) | -1 | -1 |
| G: -6727.38569 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12992.66895 HOMO: -7.21646 LUMO: -1.53472 factor:1 | 1 (-0.91757) | -1 | -1 |
| G: -6727.38569 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12992.93927 HOMO: -6.73754 LUMO: -1.37417 factor:1 | 1 (-1.18789) | -1 | -1 |
| G: -6727.38569 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12992.96441 HOMO: -6.78924 LUMO: 0.66396 factor:1 | 1 (-1.21303) | -1 | -1 |
| G: -6727.38569 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12993.05720 HOMO: -6.82734 LUMO: 0.61226 factor:1 | 1 (-1.30582) | -1 | -1 |
| G: -6727.38569 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12992.96289 HOMO: -6.74026 LUMO: 0.65579 factor:1 | 1 (-1.21151) | -1 | -1 |
| G: -6727.38569 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12993.13761 HOMO: -7.10489 LUMO: -1.30887 factor:1 | 1 (-1.38623) | -1 | -1 |
| G: -6727.38569 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12993.08324 HOMO: -7.05047 LUMO: 0.42722 factor:1 | 1 (-1.33186) | -1 | -1 |
| G: -6727.38569 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12993.07402 HOMO: -6.61237 LUMO: 1.30887 factor:1 | 1 (-1.32264) | -1 | -1 |
| G: -6727.38569 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12993.14670 HOMO: -7.05863 LUMO: 0.59049 factor:1 | 1 (-1.39532) | -1 | -1 |
| G: -6727.38569 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12992.95418 HOMO: -6.26406 LUMO: 0.78641 factor:1 | 1 (-1.20280) | -1 | -1 |
| G: -6727.38569 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12992.95040 HOMO: -6.70489 LUMO: 0.67756 factor:1 | 1 (-1.19902) | -1 | -1 |
| G: -6727.38569 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12993.12912 HOMO: -6.78652 LUMO: -0.94968 factor:1 | 1 (-1.37774) | -1 | -1 |
| G: -6727.38569 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12993.10234 HOMO: -6.36202 LUMO: -0.94424 factor:1 | 1 (-1.35096) | -1 | -1 |
| G: -6727.38569 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12993.22684 HOMO: -6.81645 LUMO: -1.09934 factor:1 | 1 (-1.47546) | -1 | -1 |
| G: -6727.38569 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12991.83342 HOMO: -7.07224 LUMO: 0.85988 factor:1 | 1 (-0.08204) | 1 | 1 |
| G: -6727.38569 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12992.73692 HOMO: -7.02326 LUMO: 1.10206 factor:1 | 1 (-0.98554) | -1 | -1 |
| G: -6727.38569 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12993.36311 HOMO: -6.71305 LUMO: 0.84627 factor:1 | 1 (-1.61173) | -1 | -1 |
| G: -6727.38569 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12993.15456 HOMO: -7.27360 LUMO: 0.88165 factor:1 | 1 (-1.40318) | 1 | 1 |
| G: -6727.38569 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12991.96494 HOMO: -6.84911 LUMO: 0.59865 factor:1 | 1 (-0.21355) | -1 | -1 |
| G: -6727.38569 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12992.24483 HOMO: -6.75114 LUMO: -2.49801 factor:1 | 1 (-0.49345) | -1 | -1 |
| G: -6727.38569 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12992.74364 HOMO: -6.97156 LUMO: 0.53606 factor:1 | 1 (-0.99226) | -1 | -1 |
| G: -6727.38569 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12993.31473 HOMO: -6.54434 LUMO: 0.73199 factor:1 | 1 (-1.56335) | -1 | -1 |
| G: -6727.38569 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12992.81997 HOMO: -6.21236 LUMO: 0.99866 factor:1 | 1 (-1.06859) | -1 | -1 |
| G: -6727.38569 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12993.18172 HOMO: -6.34025 LUMO: 0.50341 factor:1 | 1 (-1.43034) | -1 | -1 |
| G: -6727.38569 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12991.93666 HOMO: -6.59876 LUMO: -0.69389 factor:1 | 1 (-0.18528) | -1 | -1 |
| G: -6727.38569 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12992.02654 HOMO: -6.54978 LUMO: -1.00682 factor:1 | 1 (-0.27516) | -1 | -1 |
| G: -6727.38569 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12992.69602 HOMO: -6.82462 LUMO: -0.98777 factor:1 | 1 (-0.94464) | -1 | -1 |
| G: -6727.38569 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12992.91317 HOMO: -6.85455 LUMO: -0.68573 factor:1 | 1 (-1.16179) | -1 | -1 |
| G: -6727.38569 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12992.66057 HOMO: -7.55388 LUMO: -0.03265 factor:1 | 1 (-0.90919) | 1 | 1 |
| G: -6727.38569 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12992.14464 HOMO: -6.77019 LUMO: -0.71838 factor:1 | 1 (-0.39326) | -1 | -1 |
| G: -6727.38569 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12993.40747 HOMO: -6.84911 LUMO: -1.25444 factor:1 | 1 (-1.65608) | -1 | -1 |
| G: -6727.38569 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12992.72620 HOMO: -6.95251 LUMO: -1.03675 factor:1 | 1 (-0.97482) | -1 | -1 |
| G: -6727.38569 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12993.27057 HOMO: -6.80829 LUMO: -0.77280 factor:1 | 1 (-1.51918) | -1 | -1 |
| G: -6727.38569 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12992.74313 HOMO: -6.94162 LUMO: -0.94151 factor:1 | 1 (-0.99175) | -1 | -1 |
| G: -6727.38569 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12992.51137 HOMO: -6.89809 LUMO: -0.90886 factor:1 | 1 (-0.75999) | -1 | -1 |
| G: -6727.38569 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12992.96044 HOMO: -6.85183 LUMO: -0.88981 factor:1 | 1 (-1.20906) | -1 | -1 |
| G: -6727.38569 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12992.61692 HOMO: -6.51985 LUMO: -0.84627 factor:1 | 1 (-0.86554) | -1 | -1 |
| G: -6727.38569 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12993.48921 HOMO: -6.83278 LUMO: -1.08029 factor:1 | 1 (-1.73783) | -1 | -1 |
| G: -6727.38569 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12992.50769 HOMO: -6.91986 LUMO: 0.66396 factor:1 | 1 (-0.75631) | -1 | -1 |
| G: -6727.38569 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12990.37307 HOMO: -6.94162 LUMO: 0.50885 factor:1 | -1 (1.37831) | -1 | -1 |
| G: -6727.38569 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12992.87396 HOMO: -6.94435 LUMO: 0.80546 factor:1 | 1 (-1.12258) | -1 | -1 |
| G: -6727.38569 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12992.96670 HOMO: -6.74298 LUMO: -0.81634 factor:1 | 1 (-1.21531) | -1 | -1 |
| G: -6727.38569 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12992.62146 HOMO: -7.04503 LUMO: 1.15921 factor:1 | 1 (-0.87008) | -1 | -1 |
| G: -6727.38569 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12991.69704 HOMO: -6.76475 LUMO: 0.75920 factor:1 | -1 (0.05434) | -1 | -1 |
| G: -6727.83236 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12991.26024 HOMO: -7.05047 LUMO: 0.68845 factor:1 | -1 (0.93781) | -1 | -1 |
| G: -6727.83236 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12991.00976 HOMO: -7.12666 LUMO: 0.60681 factor:1 | -1 (1.18829) | 1 | 1 |
| G: -6727.83236 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12991.13880 HOMO: -6.90897 LUMO: -1.22723 factor:1 | -1 (1.05926) | -1 | -1 |
| G: -6727.83236 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12990.82383 HOMO: -7.10761 LUMO: 0.58232 factor:1 | -1 (1.37423) | 1 | 1 |
| G: -6727.83236 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12990.59914 HOMO: -6.57427 LUMO: 0.71294 factor:1 | -1 (1.59891) | -1 | -1 |
| G: -6727.83236 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12990.85749 HOMO: -6.22597 LUMO: 0.99322 factor:1 | -1 (1.34057) | -1 | -1 |
| G: -6727.83236 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12990.88976 HOMO: -6.83550 LUMO: -0.77825 factor:1 | -1 (1.30830) | -1 | -1 |
| G: -6727.83236 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12990.95806 HOMO: -7.14843 LUMO: 0.44627 factor:1 | -1 (1.24000) | 1 | 1 |
| G: -6727.83236 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12990.85215 HOMO: -7.08040 LUMO: 0.78913 factor:1 | -1 (1.34590) | 1 | 1 |
| G: -6727.83236 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12991.17102 HOMO: -6.81373 LUMO: -0.93879 factor:1 | -1 (1.02704) | -1 | -1 |
| G: -6727.83236 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12990.83561 HOMO: -6.95251 LUMO: 0.22585 factor:1 | -1 (1.36245) | -1 | -1 |
| G: -6727.83236 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12991.02775 HOMO: -7.13483 LUMO: -1.25444 factor:1 | -1 (1.17031) | -1 | -1 |
| G: -6727.83236 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12990.63471 HOMO: -6.37835 LUMO: -1.54289 factor:1 | -1 (1.56335) | -1 | -1 |
| G: -6727.83236 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12990.80219 HOMO: -6.53617 LUMO: -1.43948 factor:1 | -1 (1.39586) | -1 | -1 |
| G: -6727.83236 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12990.98786 HOMO: -6.38379 LUMO: 0.16055 factor:1 | -1 (1.21020) | -1 | -1 |
| G: -6727.83236 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12990.84347 HOMO: -6.53617 LUMO: 0.15783 factor:1 | -1 (1.35458) | -1 | -1 |
| G: -6727.83236 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12993.82026 HOMO: -6.79740 LUMO: -0.17960 factor:1 | 1 (-1.62221) | -1 | -1 |
| G: -6727.83236 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12993.33114 HOMO: -6.26678 LUMO: -0.41361 factor:1 | 1 (-1.13308) | -1 | -1 |
| G: -6727.83236 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12993.38417 HOMO: -6.35658 LUMO: -0.24218 factor:1 | 1 (-1.18612) | -1 | -1 |
| G: -6727.83236 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12993.53280 HOMO: -6.48175 LUMO: -0.71566 factor:1 | 1 (-1.33475) | -1 | -1 |
| G: -6727.83236 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12993.40551 HOMO: -6.21508 LUMO: -0.40001 factor:1 | 1 (-1.20745) | -1 | -1 |
| G: -6727.83236 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12993.41383 HOMO: -6.51985 LUMO: -0.32654 factor:1 | 1 (-1.21578) | -1 | -1 |
| G: -6727.83236 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12993.43702 HOMO: -6.45182 LUMO: -0.66396 factor:1 | 1 (-1.23896) | -1 | -1 |
| G: -6727.83236 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12993.32866 HOMO: -6.51441 LUMO: -0.65307 factor:1 | 1 (-1.13061) | -1 | -1 |
| G: -6727.83236 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12993.79060 HOMO: -6.57971 LUMO: -0.92519 factor:1 | 1 (-1.59255) | -1 | -1 |
| G: -6727.83236 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12993.27301 HOMO: -6.67223 LUMO: -0.58232 factor:1 | 1 (-1.07496) | -1 | -1 |
| G: -6727.83236 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12993.24926 HOMO: -6.10351 LUMO: -0.45987 factor:1 | 1 (-1.05120) | -1 | -1 |
| G: -6727.83236 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12992.94465 HOMO: -6.13889 LUMO: -0.50341 factor:1 | 1 (-0.74660) | -1 | -1 |
| G: -6727.83236 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12992.08826 HOMO: -6.63141 LUMO: -0.28300 factor:1 | -1 (0.10980) | -1 | -1 |
| G: -6727.83236 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12993.43424 HOMO: -6.37563 LUMO: -0.22858 factor:1 | 1 (-1.23619) | -1 | -1 |
| G: -6727.83236 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12993.31723 HOMO: -6.37019 LUMO: 0.11429 factor:1 | 1 (-1.11918) | -1 | -1 |
| G: -6727.83236 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12993.41081 HOMO: -6.23957 LUMO: 0.28844 factor:1 | 1 (-1.21276) | -1 | -1 |
| G: -6727.83236 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12992.00246 HOMO: -6.41372 LUMO: -0.53879 factor:1 | -1 (0.19560) | -1 | -1 |
| G: -6727.83236 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12992.89241 HOMO: -7.06680 LUMO: 0.32654 factor:1 | 1 (-0.69435) | 1 | 1 |
| G: -6727.83236 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12993.66072 HOMO: -6.50896 LUMO: -0.73743 factor:1 | 1 (-1.46267) | -1 | -1 |
| G: -6727.83236 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12993.11024 HOMO: -6.42189 LUMO: -0.28572 factor:1 | 1 (-0.91218) | -1 | -1 |
| G: -6727.83236 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12992.98642 HOMO: -6.79740 LUMO: -0.25851 factor:1 | 1 (-0.78837) | -1 | -1 |
| G: -6727.83236 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12993.20817 HOMO: -6.32393 LUMO: 0.17960 factor:1 | 1 (-1.01011) | -1 | -1 |
| G: -6727.83236 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12992.98593 HOMO: -6.65046 LUMO: 0.03537 factor:1 | 1 (-0.78788) | -1 | -1 |
| G: -6727.83236 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12993.19535 HOMO: -6.60148 LUMO: 0.07619 factor:1 | 1 (-0.99730) | -1 | -1 |
| G: -6727.83236 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12993.06724 HOMO: -6.57971 LUMO: 0.11429 factor:1 | 1 (-0.86919) | -1 | -1 |
| G: -6727.83236 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12993.17954 HOMO: -6.88448 LUMO: -1.21907 factor:1 | 1 (-0.98149) | -1 | -1 |
| G: -6727.83236 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12993.11247 HOMO: -6.97700 LUMO: 0.36463 factor:1 | 1 (-0.91441) | -1 | -1 |
| G: -6727.83236 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12993.62935 HOMO: -6.73210 LUMO: -0.84083 factor:1 | 1 (-1.43129) | -1 | -1 |
| G: -6727.83236 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12993.54472 HOMO: -6.21236 LUMO: -0.68845 factor:1 | 1 (-1.34666) | -1 | -1 |
| G: -6727.83236 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12993.28327 HOMO: -6.35658 LUMO: -0.82995 factor:1 | 1 (-1.08522) | -1 | -1 |
| G: -6727.83236 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12993.34336 HOMO: -6.75114 LUMO: -0.94424 factor:1 | 1 (-1.14530) | -1 | -1 |
| G: -6727.83236 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12993.11285 HOMO: -6.74026 LUMO: -1.46125 factor:1 | 1 (-0.91479) | -1 | -1 |
| G: -6727.83236 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12992.65706 HOMO: -7.06952 LUMO: 0.91974 factor:1 | 1 (-0.45900) | 1 | 1 |
| G: -6727.83236 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12993.11690 HOMO: -7.08857 LUMO: 0.74559 factor:1 | 1 (-0.91885) | 1 | 1 |
| G: -6727.83236 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12993.00585 HOMO: -6.74298 LUMO: 1.03131 factor:1 | 1 (-0.80780) | -1 | -1 |
| G: -6727.83236 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12993.00974 HOMO: -6.74842 LUMO: -1.77962 factor:1 | 1 (-0.81169) | -1 | -1 |
| G: -6727.83236 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12993.59245 HOMO: -6.82462 LUMO: -1.61908 factor:1 | 1 (-1.39439) | -1 | -1 |
| G: -6727.83236 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12993.29840 HOMO: -7.17020 LUMO: -1.02043 factor:1 | 1 (-1.10035) | -1 | -1 |
| G: -6727.83236 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12993.36477 HOMO: -6.26406 LUMO: -0.96328 factor:1 | 1 (-1.16672) | -1 | -1 |
| G: -6727.83236 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12993.29187 HOMO: -6.50896 LUMO: -0.38640 factor:1 | 1 (-1.09382) | -1 | -1 |
| G: -6727.83236 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12992.96313 HOMO: -7.27632 LUMO: -1.17553 factor:1 | 1 (-0.76508) | -1 | -1 |
| G: -6727.83236 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12992.07743 HOMO: -6.54162 LUMO: -1.36873 factor:1 | -1 (0.12063) | -1 | -1 |
| G: -6727.83236 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12993.25622 HOMO: -6.42733 LUMO: -1.15648 factor:1 | 1 (-1.05817) | -1 | -1 |
| G: -6727.83236 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12993.07021 HOMO: -6.73754 LUMO: -2.58780 factor:1 | 1 (-0.87215) | -1 | -1 |
| G: -6727.83236 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12993.29606 HOMO: -7.20285 LUMO: 0.75103 factor:1 | 1 (-1.09801) | 1 | 1 |
| G: -6727.83236 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12993.26376 HOMO: -6.98788 LUMO: 0.34831 factor:1 | 1 (-1.06571) | -1 | -1 |
| G: -6727.83236 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12993.29799 HOMO: -6.80013 LUMO: -1.11567 factor:1 | 1 (-1.09994) | -1 | -1 |
| G: -6727.83236 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12992.99954 HOMO: -6.67767 LUMO: -0.82450 factor:1 | 1 (-0.80148) | -1 | -1 |
| G: -6727.83236 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12993.00226 HOMO: -6.84911 LUMO: -0.21497 factor:1 | 1 (-0.80421) | -1 | -1 |
| G: -6727.83236 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12992.84193 HOMO: -6.23141 LUMO: 0.21769 factor:1 | 1 (-0.64388) | -1 | -1 |
| G: -6727.83236 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12991.03578 HOMO: -6.68312 LUMO: 0.16327 factor:1 | -1 (1.16228) | -1 | -1 |
| G: -6727.83236 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12992.69330 HOMO: -7.04503 LUMO: -1.04220 factor:1 | 1 (-0.49525) | -1 | -1 |
| G: -6727.83236 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12991.86137 HOMO: -6.67495 LUMO: -0.71294 factor:1 | -1 (0.33669) | -1 | -1 |
| G: -6727.83236 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12992.75507 HOMO: -6.70216 LUMO: -0.55239 factor:1 | 1 (-0.55702) | -1 | -1 |
| G: -6727.83236 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12993.18063 HOMO: -6.60420 LUMO: -0.71294 factor:1 | 1 (-0.98258) | -1 | -1 |
| G: -6727.83236 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12993.27916 HOMO: -7.40694 LUMO: 0.11973 factor:1 | 1 (-1.08111) | 1 | 1 |
| G: -6727.83236 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12993.12836 HOMO: -6.58788 LUMO: -0.29116 factor:1 | 1 (-0.93030) | -1 | -1 |
| G: -6727.83236 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12991.14900 HOMO: -6.63686 LUMO: -0.32654 factor:1 | -1 (1.04905) | -1 | -1 |
| G: -6727.83236 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12993.09715 HOMO: -6.85183 LUMO: -0.95512 factor:1 | 1 (-0.89909) | -1 | -1 |
| G: -6727.83236 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12993.17005 HOMO: -6.82189 LUMO: -0.88165 factor:1 | 1 (-0.97199) | -1 | -1 |
| G: -6727.83236 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12993.44227 HOMO: -6.97428 LUMO: -1.03947 factor:1 | 1 (-1.24421) | -1 | -1 |
| G: -6727.83236 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12993.27769 HOMO: -6.51441 LUMO: -0.05714 factor:1 | 1 (-1.07964) | -1 | -1 |
| G: -6727.83236 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12993.41508 HOMO: -6.61509 LUMO: -0.77008 factor:1 | 1 (-1.21703) | -1 | -1 |
| G: -6727.83236 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12993.06185 HOMO: -7.36340 LUMO: 0.29116 factor:1 | 1 (-0.86380) | 1 | 1 |
| G: -6727.83236 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12993.03415 HOMO: -6.64230 LUMO: -0.79185 factor:1 | 1 (-0.83610) | -1 | -1 |
| G: -6727.83236 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12993.13391 HOMO: -6.56883 LUMO: -1.03403 factor:1 | 1 (-0.93585) | -1 | -1 |
| G: -6727.83236 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12990.99431 HOMO: -6.69400 LUMO: -0.77825 factor:1 | -1 (1.20375) | -1 | -1 |
| G: -6727.83236 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12992.84332 HOMO: -6.37019 LUMO: -0.79185 factor:1 | 1 (-0.64526) | -1 | -1 |
| G: -6727.83236 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12992.05378 HOMO: -6.49808 LUMO: -0.94424 factor:1 | -1 (0.14427) | -1 | -1 |
| G: -6727.83236 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12990.96519 HOMO: -6.91713 LUMO: -0.75376 factor:1 | -1 (1.23287) | -1 | -1 |
| G: -6727.83236 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12991.02495 HOMO: -7.13755 LUMO: 0.41361 factor:1 | -1 (1.17311) | 1 | 1 |
| G: -6727.83236 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12993.10591 HOMO: -7.12122 LUMO: 0.39457 factor:1 | 1 (-0.90785) | 1 | 1 |
| G: -6727.83236 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12992.31594 HOMO: -6.59332 LUMO: -0.57144 factor:1 | 1 (-0.11788) | -1 | -1 |
| G: -6727.83236 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12993.09015 HOMO: -6.62325 LUMO: -0.66940 factor:1 | 1 (-0.89210) | -1 | -1 |
| G: -6727.83236 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12993.05407 HOMO: -6.90897 LUMO: -0.08708 factor:1 | 1 (-0.85602) | -1 | -1 |
| G: -6727.83236 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12993.55144 HOMO: -6.65591 LUMO: -0.81090 factor:1 | 1 (-1.35339) | -1 | -1 |
| G: -6727.83236 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12992.24491 HOMO: -6.65318 LUMO: -0.94696 factor:1 | 1 (-0.04686) | -1 | -1 |
| G: -6727.83236 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12992.36192 HOMO: -6.96067 LUMO: -1.03675 factor:1 | 1 (-0.16387) | -1 | -1 |
| G: -6727.83236 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12993.44853 HOMO: -6.23141 LUMO: -0.66396 factor:1 | 1 (-1.25047) | -1 | -1 |
| G: -6727.83236 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12992.65480 HOMO: -6.52529 LUMO: -0.78369 factor:1 | 1 (-0.45674) | -1 | -1 |
| G: -6727.83236 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12992.41920 HOMO: -6.39468 LUMO: -0.40817 factor:1 | 1 (-0.22115) | -1 | -1 |
| G: -6727.83236 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12993.13551 HOMO: -6.76203 LUMO: -0.20409 factor:1 | 1 (-0.93746) | -1 | -1 |
| G: -6727.83236 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12993.06996 HOMO: -6.96611 LUMO: -0.90342 factor:1 | 1 (-0.87191) | -1 | -1 |
| G: -6727.83236 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12993.50573 HOMO: -6.54706 LUMO: -0.87893 factor:1 | 1 (-1.30767) | -1 | -1 |
| G: -6727.83236 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12992.97772 HOMO: -7.24367 LUMO: -0.97689 factor:1 | 1 (-0.77966) | -1 | -1 |
| G: -6727.83236 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12992.87782 HOMO: -6.61781 LUMO: 1.43404 factor:1 | 1 (-0.67977) | -1 | -1 |
| G: -6727.83236 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12993.63122 HOMO: -6.17971 LUMO: 1.79867 factor:1 | 1 (-1.43317) | -1 | -1 |
| G: -6727.83236 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12993.33084 HOMO: -5.73344 LUMO: 2.13609 factor:1 | 1 (-1.13278) | -1 | -1 |
| G: -6727.83236 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12993.17998 HOMO: -6.72121 LUMO: 2.06807 factor:1 | 1 (-0.98192) | -1 | -1 |
| G: -6727.83236 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12993.17105 HOMO: -6.91169 LUMO: 2.02997 factor:1 | 1 (-0.97300) | -1 | -1 |
| G: -6727.83236 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12990.46842 HOMO: -7.06408 LUMO: 1.41499 factor:1 | -1 (1.72964) | 1 | 1 |
| G: -6727.83236 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12991.77124 HOMO: -6.94162 LUMO: -0.90070 factor:1 | -1 (0.42681) | -1 | -1 |
| G: -6727.83236 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12992.74949 HOMO: -7.09401 LUMO: 0.35103 factor:1 | 1 (-0.55144) | 1 | 1 |
| G: -6727.83236 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12991.97919 HOMO: -6.78652 LUMO: 0.91974 factor:1 | -1 (0.21886) | -1 | -1 |
| G: -6727.83236 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12992.92392 HOMO: -6.32937 LUMO: -1.89119 factor:1 | 1 (-0.72586) | -1 | -1 |
| G: -6727.83236 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12992.77167 HOMO: -7.12666 LUMO: -1.06397 factor:1 | 1 (-0.57362) | -1 | -1 |
| G: -6727.83236 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12992.54832 HOMO: -6.38107 LUMO: -1.43132 factor:1 | 1 (-0.35026) | -1 | -1 |
| G: -6727.83236 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12992.08268 HOMO: -7.09129 LUMO: 0.08980 factor:1 | -1 (0.11538) | 1 | 1 |
| G: -6727.83236 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12991.77650 HOMO: -6.31304 LUMO: -0.57960 factor:1 | -1 (0.42156) | -1 | -1 |
| G: -6727.83236 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12992.49330 HOMO: -6.94435 LUMO: -0.74287 factor:1 | 1 (-0.29524) | -1 | -1 |
| G: -6727.83236 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12992.24053 HOMO: -6.35658 LUMO: -1.53472 factor:1 | 1 (-0.04248) | -1 | -1 |
| G: -6727.83236 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12993.12762 HOMO: -6.39740 LUMO: -1.48846 factor:1 | 1 (-0.92957) | -1 | -1 |
| G: -6727.83236 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12993.64965 HOMO: -7.05319 LUMO: -0.33198 factor:1 | 1 (-1.45159) | -1 | -1 |
| G: -6727.83236 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12993.01551 HOMO: -6.68040 LUMO: -0.09252 factor:1 | 1 (-0.81746) | -1 | -1 |
| G: -6727.83236 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12990.76614 HOMO: -6.35930 LUMO: -0.43266 factor:1 | -1 (1.43192) | -1 | -1 |
| G: -6727.83236 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12992.87834 HOMO: -6.59604 LUMO: -1.45853 factor:1 | 1 (-0.68028) | -1 | -1 |
| G: -6727.83236 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12993.01826 HOMO: -6.46270 LUMO: -1.49391 factor:1 | 1 (-0.82021) | -1 | -1 |
| G: -6727.83236 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12990.72959 HOMO: -7.05863 LUMO: -1.04764 factor:1 | -1 (1.46846) | -1 | -1 |
| G: -6727.83236 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12992.02241 HOMO: -7.14027 LUMO: -0.81634 factor:1 | -1 (0.17565) | -1 | -1 |
| G: -6727.83236 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12992.57039 HOMO: -6.80285 LUMO: -0.74287 factor:1 | 1 (-0.37233) | -1 | -1 |
| G: -6727.83236 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12991.61799 HOMO: -6.53890 LUMO: -1.13471 factor:1 | -1 (0.58007) | -1 | -1 |
| G: -6727.83236 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12992.67488 HOMO: -6.49808 LUMO: -1.35513 factor:1 | 1 (-0.47683) | -1 | -1 |
| G: -6727.83236 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12991.78284 HOMO: -6.75931 LUMO: -1.49663 factor:1 | -1 (0.41522) | -1 | -1 |
| G: -6727.83236 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12992.97494 HOMO: -6.84638 LUMO: -0.77552 factor:1 | 1 (-0.77689) | -1 | -1 |
| G: -6727.83236 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12992.06281 HOMO: -6.65863 LUMO: -1.34696 factor:1 | -1 (0.13524) | -1 | -1 |
| G: -6727.83236 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12990.93988 HOMO: -6.25590 LUMO: -2.36467 factor:1 | -1 (1.25817) | -1 | -1 |
| G: -6727.83236 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12991.76104 HOMO: -7.24911 LUMO: 0.33470 factor:1 | -1 (0.43701) | 1 | 1 |
| G: -6727.83236 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12991.88801 HOMO: -6.65863 LUMO: -0.75648 factor:1 | -1 (0.31005) | -1 | -1 |
| G: -6727.83236 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12993.23443 HOMO: -6.31576 LUMO: -0.83267 factor:1 | 1 (-1.03637) | -1 | -1 |
| G: -6727.83236 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12992.35153 HOMO: -6.64774 LUMO: -0.66124 factor:1 | 1 (-0.15347) | -1 | -1 |
| G: -6727.83236 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12993.11356 HOMO: -6.75387 LUMO: -1.00138 factor:1 | 1 (-0.91550) | -1 | -1 |
| G: -6727.83236 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12993.20670 HOMO: -6.52529 LUMO: -0.68301 factor:1 | 1 (-1.00864) | -1 | -1 |
| G: -6727.83236 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12993.31106 HOMO: -6.59332 LUMO: -0.68028 factor:1 | 1 (-1.11300) | -1 | -1 |
| G: -6727.83236 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12993.33119 HOMO: -5.98650 LUMO: 0.31565 factor:1 | 1 (-1.13314) | -1 | -1 |
| G: -6727.83236 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12993.19456 HOMO: -6.59876 LUMO: 0.22585 factor:1 | 1 (-0.99651) | -1 | -1 |
| G: -6727.83236 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12993.02313 HOMO: -6.72121 LUMO: 0.10340 factor:1 | 1 (-0.82508) | -1 | -1 |
| G: -6727.83236 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12993.10030 HOMO: -6.09807 LUMO: 0.20136 factor:1 | 1 (-0.90225) | -1 | -1 |
| G: -6727.83236 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12992.79978 HOMO: -6.31576 LUMO: 0.06259 factor:1 | 1 (-0.60173) | -1 | -1 |
| G: -6727.83236 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12993.03954 HOMO: -6.35658 LUMO: -0.58232 factor:1 | 1 (-0.84148) | -1 | -1 |
| G: -6727.83236 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12992.93401 HOMO: -6.34842 LUMO: -0.55783 factor:1 | 1 (-0.73596) | -1 | -1 |
| G: -6727.83236 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12992.31057 HOMO: -6.47359 LUMO: -0.57144 factor:1 | 1 (-0.11252) | -1 | -1 |
| G: -6727.83236 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12992.81848 HOMO: -6.42189 LUMO: -0.09796 factor:1 | 1 (-0.62042) | -1 | -1 |
| G: -6727.83236 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12993.14000 HOMO: -6.35658 LUMO: -0.31293 factor:1 | 1 (-0.94195) | -1 | -1 |
| G: -6727.83236 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12992.60623 HOMO: -7.35524 LUMO: 0.10340 factor:1 | 1 (-0.40817) | 1 | 1 |
| G: -6727.83236 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12991.90210 HOMO: -7.10217 LUMO: 0.36463 factor:1 | -1 (0.29595) | 1 | 1 |
| G: -6727.83236 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12993.60796 HOMO: -6.43549 LUMO: -0.56872 factor:1 | 1 (-1.40990) | -1 | -1 |
| G: -6727.83236 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12992.70206 HOMO: -6.50080 LUMO: -0.71294 factor:1 | 1 (-0.50401) | -1 | -1 |
| G: -6727.83236 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12993.02501 HOMO: -6.59060 LUMO: -0.57960 factor:1 | 1 (-0.82695) | -1 | -1 |
| G: -6727.83236 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12993.36831 HOMO: -6.78924 LUMO: -0.31565 factor:1 | 1 (-1.17025) | -1 | -1 |
| G: -6727.83236 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12993.01083 HOMO: -6.35658 LUMO: 0.07891 factor:1 | 1 (-0.81278) | -1 | -1 |
| G: -6727.83236 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12993.01415 HOMO: -6.74026 LUMO: -0.87621 factor:1 | 1 (-0.81610) | -1 | -1 |
| G: -6727.83236 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12993.11132 HOMO: -6.54434 LUMO: 0.81906 factor:1 | 1 (-0.91327) | -1 | -1 |
| G: -6727.83236 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12993.13007 HOMO: -6.66135 LUMO: 1.40955 factor:1 | 1 (-0.93202) | -1 | -1 |
| G: -6727.83236 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12993.36570 HOMO: -6.73754 LUMO: -2.54971 factor:1 | 1 (-1.16764) | -1 | -1 |
| G: -6727.83236 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12992.65610 HOMO: -6.65318 LUMO: 0.69389 factor:1 | 1 (-0.45805) | -1 | -1 |
| G: -6727.83236 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12991.70724 HOMO: -6.73482 LUMO: 0.62858 factor:1 | -1 (0.49081) | -1 | -1 |
| G: -6727.83236 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12992.78435 HOMO: -6.83550 LUMO: 0.68573 factor:1 | 1 (-0.58630) | -1 | -1 |
| G: -6727.83236 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12991.81720 HOMO: -6.83278 LUMO: 0.45987 factor:1 | -1 (0.38085) | -1 | -1 |
| G: -6727.83236 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12993.11312 HOMO: -6.78380 LUMO: 0.68301 factor:1 | 1 (-0.91506) | -1 | -1 |
| G: -6727.83236 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12991.24718 HOMO: -6.90625 LUMO: 1.36601 factor:1 | -1 (0.95087) | -1 | -1 |
| G: -6727.83236 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12993.01821 HOMO: -6.82734 LUMO: 1.48302 factor:1 | 1 (-0.82015) | -1 | -1 |
| G: -6727.83236 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12992.96876 HOMO: -6.44094 LUMO: -0.94424 factor:1 | 1 (-0.77071) | -1 | -1 |
| G: -6727.83236 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12992.69676 HOMO: -6.91441 LUMO: 0.28844 factor:1 | 1 (-0.49870) | -1 | -1 |
| G: -6727.83236 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12993.08792 HOMO: -6.49808 LUMO: -0.51157 factor:1 | 1 (-0.88987) | -1 | -1 |
| G: -6727.83236 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12991.02799 HOMO: -7.09673 LUMO: -0.06259 factor:1 | -1 (1.17006) | 1 | 1 |
| G: -6727.83236 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12992.87445 HOMO: -6.77019 LUMO: 0.92247 factor:1 | 1 (-0.67639) | -1 | -1 |
| G: -6727.83236 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12992.67115 HOMO: -6.75931 LUMO: 1.13744 factor:1 | 1 (-0.47310) | -1 | -1 |
| G: -6727.83236 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12992.87434 HOMO: -6.15794 LUMO: 1.12383 factor:1 | 1 (-0.67628) | -1 | -1 |
| G: -6727.83236 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12992.77603 HOMO: -6.59604 LUMO: 1.19458 factor:1 | 1 (-0.57797) | -1 | -1 |
| G: -6727.83236 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12992.49044 HOMO: -7.09401 LUMO: 0.60137 factor:1 | 1 (-0.29239) | 1 | 1 |
| G: -6727.83236 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12992.94536 HOMO: -6.34025 LUMO: 0.48164 factor:1 | 1 (-0.74731) | -1 | -1 |
| G: -6727.83236 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12993.10311 HOMO: -6.72665 LUMO: -2.47624 factor:1 | 1 (-0.90505) | -1 | -1 |
| G: -6727.83236 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12993.23467 HOMO: -6.48175 LUMO: 0.58232 factor:1 | 1 (-1.03662) | -1 | -1 |
| G: -6727.83236 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12992.62639 HOMO: -6.94162 LUMO: 0.28300 factor:1 | 1 (-0.42833) | -1 | -1 |
| G: -6727.83236 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12991.58721 HOMO: -6.65591 LUMO: 0.57144 factor:1 | -1 (0.61084) | -1 | -1 |
| G: -6727.83236 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12992.68854 HOMO: -6.58788 LUMO: -1.03947 factor:1 | 1 (-0.49049) | -1 | -1 |
| G: -6727.83236 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12991.88932 HOMO: -7.18108 LUMO: 0.37824 factor:1 | -1 (0.30874) | 1 | 1 |
| G: -6727.83236 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12992.61099 HOMO: -6.63958 LUMO: -1.52112 factor:1 | 1 (-0.41293) | -1 | -1 |
| G: -6727.83236 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12991.88948 HOMO: -6.12528 LUMO: -0.53606 factor:1 | -1 (0.30858) | -1 | -1 |
| G: -6727.83236 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12993.00833 HOMO: -6.22324 LUMO: -0.87893 factor:1 | 1 (-0.81027) | -1 | -1 |
| G: -6727.83236 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12993.15592 HOMO: -6.62053 LUMO: -0.91974 factor:1 | 1 (-0.95787) | -1 | -1 |
| G: -6727.83236 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12993.22126 HOMO: -6.84366 LUMO: -0.83811 factor:1 | 1 (-1.02320) | -1 | -1 |
| G: -6727.83236 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12993.50766 HOMO: -7.26000 LUMO: 0.25851 factor:1 | 1 (-1.30960) | 1 | 1 |
| G: -6727.83236 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12993.51830 HOMO: -6.49536 LUMO: -0.63403 factor:1 | 1 (-1.32024) | -1 | -1 |
| G: -6727.83236 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12992.71777 HOMO: -6.45726 LUMO: -0.77825 factor:1 | 1 (-0.51971) | -1 | -1 |
| G: -6727.83236 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12992.66895 HOMO: -6.74570 LUMO: -0.75103 factor:1 | 1 (-0.47089) | -1 | -1 |
| G: -6727.83236 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12992.93927 HOMO: -7.20285 LUMO: 0.10612 factor:1 | 1 (-0.74121) | 1 | 1 |
| G: -6727.83236 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12992.96441 HOMO: -6.45182 LUMO: -0.56600 factor:1 | 1 (-0.76635) | -1 | -1 |
| G: -6727.83236 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12993.05720 HOMO: -6.83278 LUMO: -0.71838 factor:1 | 1 (-0.85915) | -1 | -1 |
| G: -6727.83236 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12992.96289 HOMO: -7.01510 LUMO: -1.09662 factor:1 | 1 (-0.76483) | -1 | -1 |
| G: -6727.83236 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12993.13761 HOMO: -6.48719 LUMO: 0.16871 factor:1 | 1 (-0.93955) | -1 | -1 |
| G: -6727.83236 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12993.08324 HOMO: -7.30898 LUMO: 0.26667 factor:1 | 1 (-0.88519) | 1 | 1 |
| G: -6727.83236 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12993.07402 HOMO: -6.68856 LUMO: -0.78641 factor:1 | 1 (-0.87596) | -1 | -1 |
| G: -6727.83236 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12993.14670 HOMO: -6.56883 LUMO: -1.00682 factor:1 | 1 (-0.94864) | -1 | -1 |
| G: -6727.83236 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12992.95418 HOMO: -6.41100 LUMO: -0.48980 factor:1 | 1 (-0.75612) | -1 | -1 |
| G: -6727.83236 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12992.95040 HOMO: -6.52257 LUMO: -0.59865 factor:1 | 1 (-0.75234) | -1 | -1 |
| G: -6727.83236 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12993.12912 HOMO: -6.63686 LUMO: -0.56055 factor:1 | 1 (-0.93106) | -1 | -1 |
| G: -6727.83236 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12993.10234 HOMO: -6.79740 LUMO: -0.75376 factor:1 | 1 (-0.90429) | -1 | -1 |
| G: -6727.83236 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12993.22684 HOMO: -5.89127 LUMO: 0.22313 factor:1 | 1 (-1.02878) | -1 | -1 |
| G: -6727.83236 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12991.83342 HOMO: -6.34842 LUMO: 0.11429 factor:1 | -1 (0.36463) | -1 | -1 |
| G: -6727.83236 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12992.73692 HOMO: -6.13617 LUMO: 1.94834 factor:1 | 1 (-0.53887) | -1 | -1 |
| G: -6727.83236 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12993.36311 HOMO: -6.50080 LUMO: 1.74153 factor:1 | 1 (-1.16506) | -1 | -1 |
| G: -6727.83236 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12993.15456 HOMO: -6.33481 LUMO: 1.68438 factor:1 | 1 (-0.95651) | -1 | -1 |
| G: -6727.83236 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12991.96494 HOMO: -6.53073 LUMO: 1.95106 factor:1 | -1 (0.23312) | -1 | -1 |
| G: -6727.83236 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12992.24483 HOMO: -6.46270 LUMO: 1.89935 factor:1 | 1 (-0.04678) | -1 | -1 |
| G: -6727.83236 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12992.74364 HOMO: -5.87222 LUMO: 1.91568 factor:1 | 1 (-0.54559) | -1 | -1 |
| G: -6727.83236 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12993.31473 HOMO: -6.07630 LUMO: 1.81500 factor:1 | 1 (-1.11667) | -1 | -1 |
| G: -6727.83236 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12992.81997 HOMO: -6.20964 LUMO: 1.81500 factor:1 | 1 (-0.62192) | -1 | -1 |
| G: -6727.83236 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12993.18172 HOMO: -6.15522 LUMO: 1.90752 factor:1 | 1 (-0.98366) | -1 | -1 |
| G: -6727.83236 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12991.93666 HOMO: -6.11984 LUMO: 1.95378 factor:1 | -1 (0.26139) | -1 | -1 |
| G: -6727.83236 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12992.02654 HOMO: -6.58516 LUMO: 2.04358 factor:1 | -1 (0.17151) | -1 | -1 |
| G: -6727.83236 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12992.69602 HOMO: -7.37156 LUMO: 0.24490 factor:1 | 1 (-0.49797) | 1 | 1 |
| G: -6727.83236 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12992.91317 HOMO: -6.36474 LUMO: -0.90070 factor:1 | 1 (-0.71512) | -1 | -1 |
| G: -6727.83236 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12992.66057 HOMO: -6.43549 LUMO: -0.40817 factor:1 | 1 (-0.46251) | -1 | -1 |
| G: -6727.83236 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12992.14464 HOMO: -7.32258 LUMO: 0.29388 factor:1 | -1 (0.05342) | 1 | 1 |
| G: -6727.83236 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12993.40747 HOMO: -6.41372 LUMO: -0.20409 factor:1 | 1 (-1.20941) | -1 | -1 |
| G: -6727.83236 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12992.72620 HOMO: -7.18381 LUMO: 0.42722 factor:1 | 1 (-0.52815) | 1 | 1 |
| G: -6727.83236 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12993.27057 HOMO: -6.53890 LUMO: -0.54151 factor:1 | 1 (-1.07251) | -1 | -1 |
| G: -6727.83236 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12992.74313 HOMO: -6.61509 LUMO: 0.08708 factor:1 | 1 (-0.54507) | -1 | -1 |
| G: -6727.83236 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12992.51137 HOMO: -6.78108 LUMO: 2.03541 factor:1 | 1 (-0.31331) | -1 | -1 |
| G: -6727.83236 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12992.96044 HOMO: -6.50896 LUMO: 1.53472 factor:1 | 1 (-0.76238) | -1 | -1 |
| G: -6727.83236 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12992.61692 HOMO: -6.65591 LUMO: 1.80411 factor:1 | 1 (-0.41886) | -1 | -1 |
| G: -6727.83236 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12993.48921 HOMO: -6.64502 LUMO: 1.52112 factor:1 | 1 (-1.29115) | -1 | -1 |
| G: -6727.83236 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12992.50769 HOMO: -6.72938 LUMO: 1.48030 factor:1 | 1 (-0.30964) | -1 | -1 |
| G: -6727.83236 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12990.37307 HOMO: -6.16882 LUMO: 1.96466 factor:1 | -1 (1.82499) | -1 | -1 |
| G: -6727.83236 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12992.87396 HOMO: -6.22597 LUMO: 1.43132 factor:1 | 1 (-0.67590) | -1 | -1 |
| G: -6727.83236 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12992.96670 HOMO: -6.57699 LUMO: 2.05718 factor:1 | 1 (-0.76864) | -1 | -1 |
| G: -6727.83236 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12992.62146 HOMO: -6.52529 LUMO: 1.89663 factor:1 | 1 (-0.42341) | -1 | -1 |
| G: -6727.83236 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12991.69704 HOMO: -6.30760 LUMO: 1.88031 factor:1 | -1 (0.50102) | -1 | -1 |
| G: -6726.98084 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12991.26024 HOMO: -6.14977 LUMO: 1.92657 factor:1 | -1 (0.08629) | -1 | -1 |
| G: -6726.98084 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12991.00976 HOMO: -6.20964 LUMO: 1.83949 factor:1 | -1 (0.33677) | -1 | -1 |
| G: -6726.98084 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12991.13880 HOMO: -6.31848 LUMO: 1.91296 factor:1 | -1 (0.20773) | -1 | -1 |
| G: -6726.98084 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12990.82383 HOMO: -5.80691 LUMO: 2.19868 factor:1 | -1 (0.52270) | -1 | -1 |
| G: -6726.98084 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12990.59914 HOMO: -6.00827 LUMO: 2.15514 factor:1 | -1 (0.74739) | -1 | -1 |
| G: -6726.98084 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12990.85749 HOMO: -6.51713 LUMO: 2.08711 factor:1 | -1 (0.48904) | -1 | -1 |
| G: -6726.98084 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12990.88976 HOMO: -6.32937 LUMO: 2.11705 factor:1 | -1 (0.45677) | -1 | -1 |
| G: -6726.98084 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12990.95806 HOMO: -6.26678 LUMO: 1.95922 factor:1 | -1 (0.38847) | -1 | -1 |
| G: -6726.98084 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12990.85215 HOMO: -6.43005 LUMO: 2.56603 factor:1 | -1 (0.49438) | -1 | -1 |
| G: -6726.98084 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12991.17102 HOMO: -6.41644 LUMO: 2.68304 factor:1 | -1 (0.17551) | -1 | -1 |
| G: -6726.98084 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12990.83561 HOMO: -5.97834 LUMO: 2.02997 factor:1 | -1 (0.51092) | -1 | -1 |
| G: -6726.98084 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12991.02775 HOMO: -6.14161 LUMO: 1.77690 factor:1 | -1 (0.31878) | -1 | -1 |
| G: -6726.98084 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12990.63471 HOMO: -6.21508 LUMO: 1.80411 factor:1 | -1 (0.71182) | -1 | -1 |
| G: -6726.98084 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12990.80219 HOMO: -6.46270 LUMO: 2.34562 factor:1 | -1 (0.54434) | -1 | -1 |
| G: -6726.98084 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12990.98786 HOMO: -6.39195 LUMO: -0.75920 factor:1 | -1 (0.35867) | -1 | -1 |
| G: -6726.98084 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12990.84347 HOMO: -7.08584 LUMO: -1.14016 factor:1 | -1 (0.50306) | -1 | -1 |
| G: -6726.98084 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12993.82026 HOMO: -6.70216 LUMO: -0.65035 factor:1 | 1 (-2.47373) | -1 | -1 |
| G: -6726.98084 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12993.33114 HOMO: -6.79468 LUMO: -0.83811 factor:1 | 1 (-1.98461) | -1 | -1 |
| G: -6726.98084 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12993.38417 HOMO: -6.99877 LUMO: -0.79729 factor:1 | 1 (-2.03764) | -1 | -1 |
| G: -6726.98084 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12993.53280 HOMO: -7.08040 LUMO: -0.85444 factor:1 | 1 (-2.18627) | -1 | -1 |
| G: -6726.98084 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12993.40551 HOMO: -7.39333 LUMO: 0.12789 factor:1 | 1 (-2.05898) | 1 | 1 |
| G: -6726.98084 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12993.41383 HOMO: -7.05047 LUMO: 0.13878 factor:1 | 1 (-2.06730) | -1 | -1 |
| G: -6726.98084 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12993.43702 HOMO: -6.90897 LUMO: -0.77552 factor:1 | 1 (-2.09049) | -1 | -1 |
| G: -6726.98084 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12993.32866 HOMO: -7.25456 LUMO: 0.05170 factor:1 | 1 (-1.98213) | 1 | 1 |
| G: -6726.98084 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12993.79060 HOMO: -6.84638 LUMO: -0.84355 factor:1 | 1 (-2.44407) | -1 | -1 |
| G: -6726.98084 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12993.27301 HOMO: -6.78108 LUMO: -0.81634 factor:1 | 1 (-1.92648) | -1 | -1 |
| G: -6726.98084 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12993.24926 HOMO: -6.74570 LUMO: -0.77280 factor:1 | 1 (-1.90273) | -1 | -1 |
| G: -6726.98084 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12992.94465 HOMO: -7.28177 LUMO: -1.68438 factor:1 | 1 (-1.59812) | -1 | -1 |
| G: -6726.98084 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12992.08826 HOMO: -7.22190 LUMO: -1.63540 factor:1 | 1 (-0.74173) | -1 | -1 |
| G: -6726.98084 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12993.43424 HOMO: -7.15932 LUMO: -1.57554 factor:1 | 1 (-2.08771) | -1 | -1 |
| G: -6726.98084 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12993.31723 HOMO: -6.57971 LUMO: -0.93063 factor:1 | 1 (-1.97070) | -1 | -1 |
| G: -6726.98084 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12993.41081 HOMO: -6.88176 LUMO: 0.58232 factor:1 | 1 (-2.06428) | -1 | -1 |
| G: -6726.98084 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12992.00246 HOMO: -6.85727 LUMO: 0.51430 factor:1 | 1 (-0.65593) | -1 | -1 |
| G: -6726.98084 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12992.89241 HOMO: -6.83550 LUMO: 0.87893 factor:1 | 1 (-1.54588) | -1 | -1 |
| G: -6726.98084 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12993.66072 HOMO: -7.06680 LUMO: 0.87621 factor:1 | 1 (-2.31419) | 1 | 1 |
| G: -6726.98084 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12993.11024 HOMO: -6.52257 LUMO: 0.81362 factor:1 | 1 (-1.76371) | -1 | -1 |
| G: -6726.98084 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12992.98642 HOMO: -6.95523 LUMO: 1.17009 factor:1 | 1 (-1.63989) | -1 | -1 |
| G: -6726.98084 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12993.20817 HOMO: -7.21374 LUMO: 0.97145 factor:1 | 1 (-1.86164) | 1 | 1 |
| G: -6726.98084 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12992.98593 HOMO: -6.81373 LUMO: -1.54561 factor:1 | 1 (-1.63940) | -1 | -1 |
| G: -6726.98084 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12993.19535 HOMO: -6.86543 LUMO: -1.52656 factor:1 | 1 (-1.84882) | -1 | -1 |
| G: -6726.98084 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12993.06724 HOMO: -6.90081 LUMO: -0.78097 factor:1 | 1 (-1.72071) | -1 | -1 |
| G: -6726.98084 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12993.17954 HOMO: -6.64502 LUMO: -0.82723 factor:1 | 1 (-1.83301) | -1 | -1 |
| G: -6726.98084 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12993.11247 HOMO: -6.65591 LUMO: -0.82178 factor:1 | 1 (-1.76594) | -1 | -1 |
| G: -6726.98084 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12993.62935 HOMO: -6.79468 LUMO: -1.46397 factor:1 | 1 (-2.28282) | -1 | -1 |
| G: -6726.98084 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12993.54472 HOMO: -7.25728 LUMO: 0.73743 factor:1 | 1 (-2.19819) | 1 | -1 |
| G: -6726.98084 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12993.28327 HOMO: -7.00149 LUMO: 1.30070 factor:1 | 1 (-1.93674) | -1 | -1 |
| G: -6726.98084 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12993.34336 HOMO: -7.07768 LUMO: 0.78097 factor:1 | 1 (-1.99683) | 1 | -1 |
| G: -6726.98084 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12993.11285 HOMO: -6.86271 LUMO: 0.86260 factor:1 | 1 (-1.76632) | -1 | -1 |
| G: -6726.98084 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12992.65706 HOMO: -6.94707 LUMO: 0.39729 factor:1 | 1 (-1.31053) | -1 | -1 |
| G: -6726.98084 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12993.11690 HOMO: -6.79740 LUMO: 0.67484 factor:1 | 1 (-1.77037) | -1 | -1 |
| G: -6726.98084 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12993.00585 HOMO: -6.91986 LUMO: -1.14288 factor:1 | 1 (-1.65932) | -1 | -1 |
| G: -6726.98084 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12993.00974 HOMO: -6.31576 LUMO: 1.01771 factor:1 | 1 (-1.66321) | -1 | -1 |
| G: -6726.98084 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12993.59245 HOMO: -6.81645 LUMO: 0.81362 factor:1 | 1 (-2.24592) | -1 | -1 |
| G: -6726.98084 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12993.29840 HOMO: -6.92258 LUMO: -0.99594 factor:1 | 1 (-1.95187) | -1 | -1 |
| G: -6726.98084 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12993.36477 HOMO: -6.81373 LUMO: 0.61770 factor:1 | 1 (-2.01824) | -1 | -1 |
| G: -6726.98084 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12993.29187 HOMO: -7.18653 LUMO: 1.19186 factor:1 | 1 (-1.94534) | 1 | 1 |
| G: -6726.98084 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12992.96313 HOMO: -7.00693 LUMO: 0.45715 factor:1 | 1 (-1.61660) | -1 | -1 |
| G: -6726.98084 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12992.07743 HOMO: -7.11306 LUMO: 0.53334 factor:1 | 1 (-0.73090) | 1 | 1 |
| G: -6726.98084 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12993.25622 HOMO: -6.63414 LUMO: -1.64357 factor:1 | 1 (-1.90970) | -1 | -1 |
| G: -6726.98084 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12993.07021 HOMO: -6.22052 LUMO: -0.74015 factor:1 | 1 (-1.72368) | -1 | -1 |
| G: -6726.98084 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12993.29606 HOMO: -6.81101 LUMO: -0.50069 factor:1 | 1 (-1.94953) | -1 | -1 |
| G: -6726.98084 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12993.26376 HOMO: -6.71849 LUMO: -0.51974 factor:1 | 1 (-1.91723) | -1 | -1 |
| G: -6726.98084 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12993.29799 HOMO: -6.72121 LUMO: -1.77690 factor:1 | 1 (-1.95146) | -1 | -1 |
| G: -6726.98084 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12992.99954 HOMO: -6.94162 LUMO: -1.78779 factor:1 | 1 (-1.65301) | -1 | -1 |
| G: -6726.98084 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12993.00226 HOMO: -6.91169 LUMO: 0.88981 factor:1 | 1 (-1.65573) | -1 | -1 |
| G: -6726.98084 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12992.84193 HOMO: -6.97428 LUMO: 0.70750 factor:1 | 1 (-1.49540) | -1 | -1 |
| G: -6726.98084 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12991.03578 HOMO: -6.74842 LUMO: 1.15921 factor:1 | -1 (0.31075) | -1 | -1 |
| G: -6726.98084 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12992.69330 HOMO: -7.25183 LUMO: -0.99594 factor:1 | 1 (-1.34677) | -1 | -1 |
| G: -6726.98084 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12991.86137 HOMO: -6.43821 LUMO: -1.00410 factor:1 | 1 (-0.51484) | -1 | -1 |
| G: -6726.98084 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12992.75507 HOMO: -6.52257 LUMO: -0.68573 factor:1 | 1 (-1.40854) | -1 | -1 |
| G: -6726.98084 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12993.18063 HOMO: -6.60148 LUMO: -0.52518 factor:1 | 1 (-1.83410) | -1 | -1 |
| G: -6726.98084 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12993.27916 HOMO: -6.07086 LUMO: -1.39594 factor:1 | 1 (-1.93263) | -1 | -1 |
| G: -6726.98084 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12993.12836 HOMO: -6.78108 LUMO: -1.54833 factor:1 | 1 (-1.78183) | -1 | -1 |
| G: -6726.98084 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12991.14900 HOMO: -6.73482 LUMO: -1.01498 factor:1 | -1 (0.19753) | -1 | -1 |
| G: -6726.98084 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12993.09715 HOMO: -6.85183 LUMO: 1.06669 factor:1 | 1 (-1.75062) | -1 | -1 |
| G: -6726.98084 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12993.17005 HOMO: -6.98516 LUMO: 1.43948 factor:1 | 1 (-1.82352) | -1 | -1 |
| G: -6726.98084 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12993.44227 HOMO: -6.94162 LUMO: 0.79185 factor:1 | 1 (-2.09574) | -1 | -1 |
| G: -6726.98084 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12993.27769 HOMO: -6.67495 LUMO: -1.06669 factor:1 | 1 (-1.93116) | -1 | -1 |
| G: -6726.98084 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12993.41508 HOMO: -6.88720 LUMO: -1.00682 factor:1 | 1 (-2.06856) | -1 | -1 |
| G: -6726.98084 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12993.06185 HOMO: -6.85999 LUMO: -0.78097 factor:1 | 1 (-1.71532) | -1 | -1 |
| G: -6726.98084 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12993.03415 HOMO: -6.51713 LUMO: -0.89798 factor:1 | 1 (-1.68762) | -1 | -1 |
| G: -6726.98084 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12993.13391 HOMO: -6.63141 LUMO: -0.91430 factor:1 | 1 (-1.78738) | -1 | -1 |
| G: -6726.98084 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12990.99431 HOMO: -6.63414 LUMO: 0.04354 factor:1 | -1 (0.35222) | -1 | -1 |
| G: -6726.98084 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12992.84332 HOMO: -6.65046 LUMO: -0.73743 factor:1 | 1 (-1.49679) | -1 | -1 |
| G: -6726.98084 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12992.05378 HOMO: -6.73754 LUMO: -0.71838 factor:1 | 1 (-0.70725) | -1 | -1 |
| G: -6726.98084 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12990.96519 HOMO: -6.65863 LUMO: -0.60137 factor:1 | -1 (0.38134) | -1 | -1 |
| G: -6726.98084 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12991.02495 HOMO: -6.61509 LUMO: -0.47892 factor:1 | -1 (0.32158) | -1 | -1 |
| G: -6726.98084 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12993.10591 HOMO: -6.82189 LUMO: -0.64763 factor:1 | 1 (-1.75938) | -1 | -1 |
| G: -6726.98084 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12992.31594 HOMO: -6.56883 LUMO: -0.51974 factor:1 | 1 (-0.96941) | -1 | -1 |
| G: -6726.98084 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12993.09015 HOMO: -6.97428 LUMO: -0.95512 factor:1 | 1 (-1.74362) | -1 | -1 |
| G: -6726.98084 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12993.05407 HOMO: -6.70489 LUMO: -0.04082 factor:1 | 1 (-1.70754) | -1 | -1 |
| G: -6726.98084 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12993.55144 HOMO: -6.74026 LUMO: 0.02177 factor:1 | 1 (-2.20491) | -1 | -1 |
| G: -6726.98084 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12992.24491 HOMO: -6.50080 LUMO: -0.89525 factor:1 | 1 (-0.89838) | -1 | -1 |
| G: -6726.98084 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12992.36192 HOMO: -6.46815 LUMO: -0.61226 factor:1 | 1 (-1.01539) | -1 | -1 |
| G: -6726.98084 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12993.44853 HOMO: -6.57971 LUMO: -0.64219 factor:1 | 1 (-2.10200) | -1 | -1 |
| G: -6726.98084 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12992.65480 HOMO: -7.17836 LUMO: 0.37280 factor:1 | 1 (-1.30827) | 1 | 1 |
| G: -6726.98084 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12992.41920 HOMO: -6.67223 LUMO: 0.12245 factor:1 | 1 (-1.07267) | -1 | -1 |
| G: -6726.98084 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12993.13551 HOMO: -6.55250 LUMO: 0.22858 factor:1 | 1 (-1.78899) | -1 | -1 |
| G: -6726.98084 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12993.06996 HOMO: -6.97156 LUMO: -1.12927 factor:1 | 1 (-1.72343) | -1 | -1 |
| G: -6726.98084 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12993.50573 HOMO: -6.78924 LUMO: -0.84900 factor:1 | 1 (-2.15920) | -1 | -1 |
| G: -6726.98084 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12992.97772 HOMO: -6.65046 LUMO: -0.65307 factor:1 | 1 (-1.63119) | -1 | -1 |
| G: -6726.98084 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12992.87782 HOMO: -7.41782 LUMO: 0.08980 factor:1 | 1 (-1.53129) | 1 | 1 |
| G: -6726.98084 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12993.63122 HOMO: -6.56339 LUMO: -0.68573 factor:1 | 1 (-2.28470) | -1 | -1 |
| G: -6726.98084 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12993.33084 HOMO: -6.31032 LUMO: -0.31837 factor:1 | 1 (-1.98431) | -1 | -1 |
| G: -6726.98084 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12993.17998 HOMO: -6.72938 LUMO: -0.45987 factor:1 | 1 (-1.83345) | -1 | -1 |
| G: -6726.98084 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12993.17105 HOMO: -6.59876 LUMO: -1.03131 factor:1 | 1 (-1.82452) | -1 | -1 |
| G: -6726.98084 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12990.46842 HOMO: -7.29265 LUMO: 0.29660 factor:1 | -1 (0.87811) | 1 | 1 |
| G: -6726.98084 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12991.77124 HOMO: -6.42189 LUMO: -0.51157 factor:1 | 1 (-0.42472) | -1 | -1 |
| G: -6726.98084 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12992.74949 HOMO: -6.27767 LUMO: -0.52790 factor:1 | 1 (-1.40296) | -1 | -1 |
| G: -6726.98084 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12991.97919 HOMO: -6.41644 LUMO: -0.44627 factor:1 | 1 (-0.63266) | -1 | -1 |
| G: -6726.98084 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12992.92392 HOMO: -6.23413 LUMO: -0.52790 factor:1 | 1 (-1.57739) | -1 | -1 |
| G: -6726.98084 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12992.77167 HOMO: -6.63414 LUMO: -0.44082 factor:1 | 1 (-1.42514) | -1 | -1 |
| G: -6726.98084 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12992.54832 HOMO: -7.03142 LUMO: 0.47076 factor:1 | 1 (-1.20179) | -1 | -1 |
| G: -6726.98084 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12992.08268 HOMO: -6.62053 LUMO: -0.14422 factor:1 | 1 (-0.73615) | -1 | -1 |
| G: -6726.98084 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12991.77650 HOMO: -6.22324 LUMO: 1.96194 factor:1 | 1 (-0.42997) | -1 | -1 |
| G: -6726.98084 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12992.49330 HOMO: -6.17971 LUMO: 1.71704 factor:1 | 1 (-1.14677) | -1 | -1 |
| G: -6726.98084 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12992.24053 HOMO: -6.70761 LUMO: 1.68711 factor:1 | 1 (-0.89400) | -1 | -1 |
| G: -6726.98084 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12993.12762 HOMO: -6.52801 LUMO: 1.56193 factor:1 | 1 (-1.78109) | -1 | -1 |
| G: -6726.98084 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12993.64965 HOMO: -6.55794 LUMO: 1.52384 factor:1 | 1 (-2.30312) | -1 | -1 |
| G: -6726.98084 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12993.01551 HOMO: -6.47359 LUMO: 1.82316 factor:1 | 1 (-1.66898) | -1 | -1 |
| G: -6726.98084 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12990.76614 HOMO: -6.65863 LUMO: 1.83133 factor:1 | -1 (0.58039) | -1 | -1 |
| G: -6726.98084 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12992.87834 HOMO: -6.46270 LUMO: 1.90208 factor:1 | 1 (-1.53181) | -1 | -1 |
| G: -6726.98084 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12993.01826 HOMO: -6.41917 LUMO: 2.03269 factor:1 | 1 (-1.67173) | -1 | -1 |
| G: -6726.98084 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12990.72959 HOMO: -6.48992 LUMO: 1.87486 factor:1 | -1 (0.61694) | -1 | -1 |
| G: -6726.98084 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12992.02241 HOMO: -6.51985 LUMO: 1.69527 factor:1 | 1 (-0.67588) | -1 | -1 |
| G: -6726.98084 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12992.57039 HOMO: -6.36202 LUMO: 2.05718 factor:1 | 1 (-1.22386) | -1 | -1 |
| G: -6726.98084 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12991.61799 HOMO: -5.96474 LUMO: 1.88575 factor:1 | 1 (-0.27146) | -1 | -1 |
| G: -6726.98084 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12992.67488 HOMO: -6.56339 LUMO: 2.04630 factor:1 | 1 (-1.32835) | -1 | -1 |
| G: -6726.98084 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12991.78284 HOMO: -6.43277 LUMO: 1.98371 factor:1 | 1 (-0.43631) | -1 | -1 |
| G: -6726.98084 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12992.97494 HOMO: -6.53345 LUMO: 2.06262 factor:1 | 1 (-1.62841) | -1 | -1 |
| G: -6726.98084 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12992.06281 HOMO: -5.81779 LUMO: 2.11432 factor:1 | 1 (-0.71629) | -1 | -1 |
| G: -6726.98084 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12990.93988 HOMO: -5.91848 LUMO: 1.86942 factor:1 | -1 (0.40665) | -1 | -1 |
| G: -6726.98084 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12991.76104 HOMO: -6.48447 LUMO: 1.70343 factor:1 | 1 (-0.41451) | -1 | -1 |
| G: -6726.98084 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12991.88801 HOMO: -6.29671 LUMO: -0.89525 factor:1 | 1 (-0.54148) | -1 | -1 |
| G: -6726.98084 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12993.23443 HOMO: -6.63414 LUMO: -0.76192 factor:1 | 1 (-1.88790) | -1 | -1 |
| G: -6726.98084 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12992.35153 HOMO: -6.56883 LUMO: -0.86260 factor:1 | 1 (-1.00500) | -1 | -1 |
| G: -6726.98084 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12993.11356 HOMO: -6.93074 LUMO: -0.27483 factor:1 | 1 (-1.76703) | -1 | -1 |
| G: -6726.98084 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12993.20670 HOMO: -6.85999 LUMO: -0.01905 factor:1 | 1 (-1.86017) | -1 | -1 |
| G: -6726.98084 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12993.31106 HOMO: -6.26406 LUMO: 0.21769 factor:1 | 1 (-1.96453) | -1 | -1 |
| G: -6726.98084 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12993.33119 HOMO: -6.62325 LUMO: 0.31293 factor:1 | 1 (-1.98466) | -1 | -1 |
| G: -6726.98084 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12993.19456 HOMO: -6.59604 LUMO: 0.19592 factor:1 | 1 (-1.84803) | -1 | -1 |
| G: -6726.98084 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12993.02313 HOMO: -6.43277 LUMO: -0.27756 factor:1 | 1 (-1.67660) | -1 | -1 |
| G: -6726.98084 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12993.10030 HOMO: -6.54978 LUMO: -0.46531 factor:1 | 1 (-1.75377) | -1 | -1 |
| G: -6726.98084 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12992.79978 HOMO: -6.65046 LUMO: -0.15783 factor:1 | 1 (-1.45325) | -1 | -1 |
| G: -6726.98084 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12993.03954 HOMO: -7.28721 LUMO: 0.23946 factor:1 | 1 (-1.69301) | 1 | 1 |
| G: -6726.98084 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12992.93401 HOMO: -6.71849 LUMO: -0.56600 factor:1 | 1 (-1.58749) | -1 | -1 |
| G: -6726.98084 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12992.31057 HOMO: -6.85183 LUMO: -0.84355 factor:1 | 1 (-0.96404) | -1 | -1 |
| G: -6726.98084 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12992.81848 HOMO: -6.53345 LUMO: -0.84627 factor:1 | 1 (-1.47195) | -1 | -1 |
| G: -6726.98084 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12993.14000 HOMO: -6.60148 LUMO: -0.63130 factor:1 | 1 (-1.79348) | -1 | -1 |
| G: -6726.98084 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12992.60623 HOMO: -6.36202 LUMO: -0.60137 factor:1 | 1 (-1.25970) | -1 | -1 |
| G: -6726.98084 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12991.90210 HOMO: -6.28855 LUMO: -0.52790 factor:1 | 1 (-0.55557) | -1 | -1 |
| G: -6726.98084 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12993.60796 HOMO: -7.07224 LUMO: 0.41906 factor:1 | 1 (-2.26143) | 1 | 1 |
| G: -6726.98084 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12992.70206 HOMO: -6.36202 LUMO: -0.24218 factor:1 | 1 (-1.35554) | -1 | -1 |
| G: -6726.98084 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12993.02501 HOMO: -6.43549 LUMO: 0.14150 factor:1 | 1 (-1.67848) | -1 | -1 |
| G: -6726.98084 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12993.36831 HOMO: -6.76747 LUMO: -0.40545 factor:1 | 1 (-2.02178) | -1 | -1 |
| G: -6726.98084 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12993.01083 HOMO: -6.15249 LUMO: -0.51157 factor:1 | 1 (-1.66430) | -1 | -1 |
| G: -6726.98084 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12993.01415 HOMO: -6.33753 LUMO: -0.02993 factor:1 | 1 (-1.66762) | -1 | -1 |
| G: -6726.98084 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12993.11132 HOMO: -6.49808 LUMO: -0.83811 factor:1 | 1 (-1.76479) | -1 | -1 |
| G: -6726.98084 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12993.13007 HOMO: -6.64502 LUMO: -0.46259 factor:1 | 1 (-1.78354) | -1 | -1 |
| G: -6726.98084 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12993.36570 HOMO: -6.34570 LUMO: 0.22041 factor:1 | 1 (-2.01917) | -1 | -1 |
| G: -6726.98084 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12992.65610 HOMO: -6.63414 LUMO: -0.13606 factor:1 | 1 (-1.30958) | -1 | -1 |
| G: -6726.98084 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12991.70724 HOMO: -6.59604 LUMO: -0.79729 factor:1 | 1 (-0.36071) | -1 | -1 |
| G: -6726.98084 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12992.78435 HOMO: -7.09401 LUMO: 0.31837 factor:1 | 1 (-1.43782) | 1 | 1 |
| G: -6726.98084 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12991.81720 HOMO: -6.48719 LUMO: -0.31021 factor:1 | 1 (-0.47068) | -1 | -1 |
| G: -6726.98084 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12993.11312 HOMO: -7.11306 LUMO: 0.39729 factor:1 | 1 (-1.76659) | 1 | 1 |
| G: -6726.98084 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12991.24718 HOMO: -6.95251 LUMO: 0.41089 factor:1 | -1 (0.09935) | -1 | -1 |
| G: -6726.98084 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12993.01821 HOMO: -6.61509 LUMO: -0.41906 factor:1 | 1 (-1.67168) | -1 | -1 |
| G: -6726.98084 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12992.96876 HOMO: -6.25318 LUMO: -0.47348 factor:1 | 1 (-1.62223) | -1 | -1 |
| G: -6726.98084 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12992.69676 HOMO: -6.77019 LUMO: -0.10340 factor:1 | 1 (-1.35023) | -1 | -1 |
| G: -6726.98084 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12993.08792 HOMO: -6.54706 LUMO: -0.46259 factor:1 | 1 (-1.74139) | -1 | -1 |
| G: -6726.98084 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12991.02799 HOMO: -6.34297 LUMO: -0.50341 factor:1 | -1 (0.31854) | -1 | -1 |
| G: -6726.98084 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12992.87445 HOMO: -6.20692 LUMO: -0.51974 factor:1 | 1 (-1.52792) | -1 | -1 |
| G: -6726.98084 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12992.67115 HOMO: -7.03686 LUMO: 0.46804 factor:1 | 1 (-1.32462) | -1 | -1 |
| G: -6726.98084 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12992.87434 HOMO: -6.47087 LUMO: 0.22585 factor:1 | 1 (-1.52781) | -1 | -1 |
| G: -6726.98084 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12992.77603 HOMO: -6.41917 LUMO: 0.19320 factor:1 | 1 (-1.42950) | -1 | -1 |
| G: -6726.98084 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12992.49044 HOMO: -6.61237 LUMO: -0.04354 factor:1 | 1 (-1.14391) | -1 | -1 |
| G: -6726.98084 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12992.94536 HOMO: -6.56339 LUMO: 0.36735 factor:1 | 1 (-1.59883) | -1 | -1 |
| G: -6726.98084 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12993.10311 HOMO: -6.54978 LUMO: 1.12655 factor:1 | 1 (-1.75658) | -1 | -1 |
| G: -6726.98084 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12993.23467 HOMO: -6.43277 LUMO: 1.17553 factor:1 | 1 (-1.88814) | -1 | -1 |
| G: -6726.98084 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12992.62639 HOMO: -6.29944 LUMO: 1.40955 factor:1 | 1 (-1.27986) | -1 | -1 |
| G: -6726.98084 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12991.58721 HOMO: -6.74842 LUMO: 0.74015 factor:1 | 1 (-0.24068) | -1 | -1 |
| G: -6726.98084 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12992.68854 HOMO: -6.15522 LUMO: 1.94289 factor:1 | 1 (-1.34201) | -1 | -1 |
| G: -6726.98084 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12991.88932 HOMO: -6.20147 LUMO: 1.40139 factor:1 | 1 (-0.54279) | -1 | -1 |
| G: -6726.98084 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12992.61099 HOMO: -6.41100 LUMO: 1.40139 factor:1 | 1 (-1.26446) | -1 | -1 |
| G: -6726.98084 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12991.88948 HOMO: -6.74570 LUMO: 1.80956 factor:1 | 1 (-0.54295) | -1 | -1 |
| G: -6726.98084 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12993.00833 HOMO: -6.60148 LUMO: -1.04764 factor:1 | 1 (-1.66180) | -1 | -1 |
| G: -6726.98084 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12993.15592 HOMO: -6.82734 LUMO: -0.83267 factor:1 | 1 (-1.80939) | -1 | -1 |
| G: -6726.98084 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12993.22126 HOMO: -7.01782 LUMO: -0.32382 factor:1 | 1 (-1.87473) | -1 | -1 |
| G: -6726.98084 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12993.50766 HOMO: -6.54434 LUMO: 0.11157 factor:1 | 1 (-2.16113) | -1 | -1 |
| G: -6726.98084 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12993.51830 HOMO: -6.53617 LUMO: 0.32926 factor:1 | 1 (-2.17177) | -1 | -1 |
| G: -6726.98084 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12992.71777 HOMO: -6.62597 LUMO: -0.60137 factor:1 | 1 (-1.37124) | -1 | -1 |
| G: -6726.98084 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12992.66895 HOMO: -6.60965 LUMO: -0.75376 factor:1 | 1 (-1.32242) | -1 | -1 |
| G: -6726.98084 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12992.93927 HOMO: -6.29399 LUMO: 0.06803 factor:1 | 1 (-1.59274) | -1 | -1 |
| G: -6726.98084 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12992.96441 HOMO: -6.60692 LUMO: -0.47076 factor:1 | 1 (-1.61788) | -1 | -1 |
| G: -6726.98084 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12993.05720 HOMO: -7.33891 LUMO: 0.39184 factor:1 | 1 (-1.71067) | 1 | 1 |
| G: -6726.98084 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12992.96289 HOMO: -6.60692 LUMO: 1.46125 factor:1 | 1 (-1.61636) | -1 | -1 |
| G: -6726.98084 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12993.13761 HOMO: -6.21780 LUMO: 2.09256 factor:1 | 1 (-1.79108) | -1 | -1 |
| G: -6726.98084 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12993.08324 HOMO: -6.28311 LUMO: 1.80411 factor:1 | 1 (-1.73671) | -1 | -1 |
| G: -6726.98084 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12993.07402 HOMO: -6.51168 LUMO: 1.84765 factor:1 | 1 (-1.72749) | -1 | -1 |
| G: -6726.98084 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12993.14670 HOMO: -6.66951 LUMO: 2.01636 factor:1 | 1 (-1.80017) | -1 | -1 |
| G: -6726.98084 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12992.95418 HOMO: -6.75387 LUMO: 1.73881 factor:1 | 1 (-1.60765) | -1 | -1 |
| G: -6726.98084 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12992.95040 HOMO: -6.77291 LUMO: 1.89935 factor:1 | 1 (-1.60387) | -1 | -1 |
| G: -6726.98084 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12993.12912 HOMO: -6.36474 LUMO: 1.61091 factor:1 | 1 (-1.78259) | -1 | -1 |
| G: -6726.98084 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12993.10234 HOMO: -6.60420 LUMO: 1.40955 factor:1 | 1 (-1.75581) | -1 | -1 |
| G: -6726.98084 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12993.22684 HOMO: -6.81645 LUMO: 1.59731 factor:1 | 1 (-1.88031) | -1 | -1 |
| G: -6726.98084 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12991.83342 HOMO: -5.90215 LUMO: 2.12249 factor:1 | 1 (-0.48689) | -1 | -1 |
| G: -6726.98084 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12992.73692 HOMO: -6.26950 LUMO: 1.62996 factor:1 | 1 (-1.39039) | -1 | -1 |
| G: -6726.98084 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12993.36311 HOMO: -6.41100 LUMO: 1.80684 factor:1 | 1 (-2.01658) | -1 | -1 |
| G: -6726.98084 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12993.15456 HOMO: -6.64230 LUMO: 2.23405 factor:1 | 1 (-1.80803) | -1 | -1 |
| G: -6726.98084 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12991.96494 HOMO: -6.66951 LUMO: 2.21501 factor:1 | 1 (-0.61841) | -1 | -1 |
| G: -6726.98084 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12992.24483 HOMO: -6.90897 LUMO: 2.00004 factor:1 | 1 (-0.89830) | -1 | -1 |
| G: -6726.98084 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12992.74364 HOMO: -6.61781 LUMO: 1.42043 factor:1 | 1 (-1.39711) | -1 | -1 |
| G: -6726.98084 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12993.31473 HOMO: -6.56611 LUMO: 1.60003 factor:1 | 1 (-1.96820) | -1 | -1 |
| G: -6726.98084 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12992.81997 HOMO: -6.70489 LUMO: 1.78779 factor:1 | 1 (-1.47344) | -1 | -1 |
| G: -6726.98084 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12993.18172 HOMO: -6.46815 LUMO: 1.59459 factor:1 | 1 (-1.83519) | -1 | -1 |
| G: -6726.98084 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12991.93666 HOMO: -6.31304 LUMO: 1.36873 factor:1 | 1 (-0.59013) | -1 | -1 |
| G: -6726.98084 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12992.02654 HOMO: -6.22597 LUMO: 1.54833 factor:1 | 1 (-0.68001) | -1 | -1 |
| G: -6726.98084 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12992.69602 HOMO: -5.63004 LUMO: 1.96466 factor:1 | 1 (-1.34949) | -1 | -1 |
| G: -6726.98084 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12992.91317 HOMO: -7.02598 LUMO: 1.79323 factor:1 | 1 (-1.56664) | -1 | -1 |
| G: -6726.98084 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12992.66057 HOMO: -6.78924 LUMO: 2.10888 factor:1 | 1 (-1.31404) | -1 | -1 |
| G: -6726.98084 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12992.14464 HOMO: -6.13345 LUMO: 2.07351 factor:1 | 1 (-0.79811) | -1 | -1 |
| G: -6726.98084 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12993.40747 HOMO: -6.46270 LUMO: -0.37552 factor:1 | 1 (-2.06094) | -1 | -1 |
| G: -6726.98084 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12992.72620 HOMO: -6.51985 LUMO: -0.49525 factor:1 | 1 (-1.37967) | -1 | -1 |
| G: -6726.98084 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12993.27057 HOMO: -6.60965 LUMO: 1.90480 factor:1 | 1 (-1.92404) | -1 | -1 |
| G: -6726.98084 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12992.74313 HOMO: -6.51168 LUMO: 1.92112 factor:1 | 1 (-1.39660) | -1 | -1 |
| G: -6726.98084 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12992.51137 HOMO: -6.71305 LUMO: 1.91024 factor:1 | 1 (-1.16484) | -1 | -1 |
| G: -6726.98084 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12992.96044 HOMO: -6.86815 LUMO: 2.02997 factor:1 | 1 (-1.61391) | -1 | -1 |
| G: -6726.98084 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12992.61692 HOMO: -6.69944 LUMO: 1.95106 factor:1 | 1 (-1.27039) | -1 | -1 |
| G: -6726.98084 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12993.48921 HOMO: -6.45182 LUMO: 1.66806 factor:1 | 1 (-2.14268) | -1 | -1 |
| G: -6726.98084 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12992.50769 HOMO: -6.44638 LUMO: 2.16058 factor:1 | 1 (-1.16116) | -1 | -1 |
| G: -6726.98084 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12990.37307 HOMO: -6.65591 LUMO: 1.95106 factor:1 | -1 (0.97346) | -1 | -1 |
| G: -6726.98084 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12992.87396 HOMO: -6.35114 LUMO: 1.42316 factor:1 | 1 (-1.52743) | -1 | -1 |
| G: -6726.98084 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12992.96670 HOMO: -6.48719 LUMO: 1.59187 factor:1 | 1 (-1.62017) | -1 | -1 |
| G: -6726.98084 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12992.62146 HOMO: -7.05591 LUMO: 1.61908 factor:1 | 1 (-1.27494) | -1 | -1 |
| G: -6726.98084 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12991.69704 HOMO: -6.92258 LUMO: 1.87214 factor:1 | 1 (-0.35051) | -1 | -1 |
| G: -6727.20729 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12991.26024 HOMO: -5.85861 LUMO: 2.11705 factor:1 | -1 (0.31274) | -1 | -1 |
| G: -6727.20729 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12991.00976 HOMO: -6.27767 LUMO: 1.75513 factor:1 | -1 (0.56322) | -1 | -1 |
| G: -6727.20729 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12991.13880 HOMO: -6.16882 LUMO: 1.73881 factor:1 | -1 (0.43418) | -1 | -1 |
| G: -6727.20729 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12990.82383 HOMO: -6.62053 LUMO: 1.39594 factor:1 | -1 (0.74916) | -1 | -1 |
| G: -6727.20729 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12990.59914 HOMO: -5.46405 LUMO: 1.68166 factor:1 | -1 (0.97384) | -1 | -1 |
| G: -6727.20729 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12990.85749 HOMO: -6.39740 LUMO: 1.68711 factor:1 | -1 (0.71550) | -1 | -1 |
| G: -6727.20729 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12990.88976 HOMO: -6.99333 LUMO: 2.08439 factor:1 | -1 (0.68322) | -1 | -1 |
| G: -6727.20729 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12990.95806 HOMO: -6.16882 LUMO: 1.71976 factor:1 | -1 (0.61492) | -1 | -1 |
| G: -6727.20729 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12990.85215 HOMO: -7.19741 LUMO: 2.24766 factor:1 | -1 (0.72083) | 1 | 1 |
| G: -6727.20729 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12991.17102 HOMO: -6.77291 LUMO: 2.17691 factor:1 | -1 (0.40197) | -1 | -1 |
| G: -6727.20729 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12990.83561 HOMO: -6.29944 LUMO: 2.16603 factor:1 | -1 (0.73737) | -1 | -1 |
| G: -6727.20729 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12991.02775 HOMO: -6.10079 LUMO: 1.83949 factor:1 | -1 (0.54523) | -1 | -1 |
| G: -6727.20729 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12990.63471 HOMO: -6.63686 LUMO: 2.05990 factor:1 | -1 (0.93828) | -1 | -1 |
| G: -6727.20729 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12990.80219 HOMO: -6.91713 LUMO: 1.87486 factor:1 | -1 (0.77079) | -1 | -1 |
| G: -6727.20729 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12990.98786 HOMO: -6.63958 LUMO: 1.79323 factor:1 | -1 (0.58513) | -1 | -1 |
| G: -6727.20729 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12990.84347 HOMO: -6.61781 LUMO: 1.70071 factor:1 | -1 (0.72951) | -1 | -1 |
| G: -6727.20729 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12993.82026 HOMO: -6.20420 LUMO: 1.82861 factor:1 | 1 (-2.24728) | -1 | -1 |
| G: -6727.20729 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12993.33114 HOMO: -6.47903 LUMO: -2.16875 factor:1 | 1 (-1.75815) | -1 | -1 |
| G: -6727.20729 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12993.38417 HOMO: -6.53073 LUMO: 2.18235 factor:1 | 1 (-1.81119) | -1 | -1 |
| G: -6727.20729 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12993.53280 HOMO: -7.01782 LUMO: 1.72520 factor:1 | 1 (-1.95982) | -1 | -1 |
| G: -6727.20729 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12993.40551 HOMO: -6.66135 LUMO: -0.75648 factor:1 | 1 (-1.83252) | -1 | -1 |
| G: -6727.20729 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12993.41383 HOMO: -7.56749 LUMO: 0.22585 factor:1 | 1 (-1.84085) | 1 | 1 |
| G: -6727.20729 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12993.43702 HOMO: -6.45182 LUMO: -0.71294 factor:1 | 1 (-1.86403) | -1 | -1 |
| G: -6727.20729 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12993.32866 HOMO: -6.31032 LUMO: -0.34286 factor:1 | 1 (-1.75568) | -1 | -1 |
| G: -6727.20729 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12993.79060 HOMO: -6.41917 LUMO: 2.04085 factor:1 | 1 (-2.21762) | -1 | -1 |
| G: -6727.20729 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12993.27301 HOMO: -6.61781 LUMO: 1.98915 factor:1 | 1 (-1.70003) | -1 | -1 |
| G: -6727.20729 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12993.24926 HOMO: -5.86405 LUMO: 1.57282 factor:1 | 1 (-1.67628) | -1 | -1 |
| G: -6727.20729 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12992.94465 HOMO: -6.44094 LUMO: 1.80956 factor:1 | 1 (-1.37167) | -1 | -1 |
| G: -6727.20729 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12992.08826 HOMO: -6.59060 LUMO: 2.08167 factor:1 | 1 (-0.51527) | -1 | -1 |
| G: -6727.20729 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12993.43424 HOMO: -6.20147 LUMO: 1.69799 factor:1 | 1 (-1.86126) | -1 | -1 |
| G: -6727.20729 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12993.31723 HOMO: -6.50352 LUMO: -0.41361 factor:1 | 1 (-1.74425) | -1 | -1 |
| G: -6727.20729 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12993.41081 HOMO: -6.10896 LUMO: -0.55783 factor:1 | 1 (-1.83783) | -1 | -1 |
| G: -6727.20729 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12992.00246 HOMO: -6.74842 LUMO: -0.56872 factor:1 | 1 (-0.42948) | -1 | -1 |
| G: -6727.20729 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12992.89241 HOMO: -6.59060 LUMO: -0.22041 factor:1 | 1 (-1.31943) | -1 | -1 |
| G: -6727.20729 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12993.66072 HOMO: -6.22052 LUMO: -0.60137 factor:1 | 1 (-2.08774) | -1 | -1 |
| G: -6727.20729 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12993.11024 HOMO: -6.65863 LUMO: 0.07891 factor:1 | 1 (-1.53725) | -1 | -1 |
| G: -6727.20729 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12992.98642 HOMO: -6.57427 LUMO: 1.71160 factor:1 | 1 (-1.41344) | -1 | -1 |
| G: -6727.20729 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12993.20817 HOMO: -5.84773 LUMO: 1.99459 factor:1 | 1 (-1.63519) | -1 | -1 |
| G: -6727.20729 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12992.98593 HOMO: -6.02188 LUMO: 1.91296 factor:1 | 1 (-1.41295) | -1 | -1 |
| G: -6727.20729 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12993.19535 HOMO: -6.17698 LUMO: 2.00004 factor:1 | 1 (-1.62237) | -1 | -1 |
| G: -6727.20729 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12993.06724 HOMO: -6.02732 LUMO: 1.90752 factor:1 | 1 (-1.49426) | -1 | -1 |
| G: -6727.20729 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12993.17954 HOMO: -6.68584 LUMO: -0.50885 factor:1 | 1 (-1.60656) | -1 | -1 |
| G: -6727.20729 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12993.11247 HOMO: -6.61781 LUMO: -0.73471 factor:1 | 1 (-1.53948) | -1 | -1 |
| G: -6727.20729 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12993.62935 HOMO: -6.66407 LUMO: -0.79729 factor:1 | 1 (-2.05636) | -1 | -1 |
| G: -6727.20729 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12993.54472 HOMO: -6.56339 LUMO: 0.23130 factor:1 | 1 (-1.97174) | -1 | -1 |
| G: -6727.20729 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12993.28327 HOMO: -6.76747 LUMO: 0.08980 factor:1 | 1 (-1.71029) | -1 | -1 |
| G: -6727.20729 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12993.34336 HOMO: -6.70489 LUMO: -0.53334 factor:1 | 1 (-1.77037) | -1 | -1 |
| G: -6727.20729 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12993.11285 HOMO: -7.28993 LUMO: 0.10885 factor:1 | 1 (-1.53987) | 1 | 1 |
| G: -6727.20729 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12992.65706 HOMO: -6.22052 LUMO: 0.51974 factor:1 | 1 (-1.08407) | -1 | -1 |
| G: -6727.20729 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12993.11690 HOMO: -6.81645 LUMO: 0.25307 factor:1 | 1 (-1.54392) | -1 | -1 |
| G: -6727.20729 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12993.00585 HOMO: -6.80285 LUMO: 0.02721 factor:1 | 1 (-1.43287) | -1 | -1 |
| G: -6727.20729 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12993.00974 HOMO: -6.51441 LUMO: 0.08163 factor:1 | 1 (-1.43676) | -1 | -1 |
| G: -6727.20729 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12993.59245 HOMO: -6.73482 LUMO: -0.77008 factor:1 | 1 (-2.01947) | -1 | -1 |
| G: -6727.20729 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12993.29840 HOMO: -6.29127 LUMO: -0.44355 factor:1 | 1 (-1.72542) | -1 | -1 |
| G: -6727.20729 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12993.36477 HOMO: -6.72938 LUMO: -0.64763 factor:1 | 1 (-1.79179) | -1 | -1 |
| G: -6727.20729 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12993.29187 HOMO: -6.49264 LUMO: -0.74559 factor:1 | 1 (-1.71889) | -1 | -1 |
| G: -6727.20729 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12992.96313 HOMO: -6.67223 LUMO: -0.55239 factor:1 | 1 (-1.39015) | -1 | -1 |
| G: -6727.20729 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12992.07743 HOMO: -6.33481 LUMO: 0.33198 factor:1 | 1 (-0.50444) | -1 | -1 |
| G: -6727.20729 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12993.25622 HOMO: -6.76475 LUMO: -0.25307 factor:1 | 1 (-1.68324) | -1 | -1 |
| G: -6727.20729 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12993.07021 HOMO: -6.65318 LUMO: 0.03810 factor:1 | 1 (-1.49722) | -1 | -1 |
| G: -6727.20729 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12993.29606 HOMO: -6.09263 LUMO: 0.21497 factor:1 | 1 (-1.72308) | -1 | -1 |
| G: -6727.20729 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12993.26376 HOMO: -6.32120 LUMO: -0.85444 factor:1 | 1 (-1.69078) | -1 | -1 |
| G: -6727.20729 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12993.29799 HOMO: -6.57155 LUMO: -0.67484 factor:1 | 1 (-1.72501) | -1 | -1 |
| G: -6727.20729 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12992.99954 HOMO: -6.53345 LUMO: -0.78913 factor:1 | 1 (-1.42656) | -1 | -1 |
| G: -6727.20729 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12993.00226 HOMO: -7.07768 LUMO: 0.28844 factor:1 | 1 (-1.42928) | 1 | 1 |
| G: -6727.20729 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12992.84193 HOMO: -6.75114 LUMO: 0.18776 factor:1 | 1 (-1.26895) | -1 | -1 |
| G: -6727.20729 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12991.03578 HOMO: -6.77019 LUMO: -0.12245 factor:1 | -1 (0.53721) | -1 | -1 |
| G: -6727.20729 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12992.69330 HOMO: -6.43549 LUMO: 0.16327 factor:1 | 1 (-1.12032) | -1 | -1 |
| G: -6727.20729 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12991.86137 HOMO: -6.69400 LUMO: -0.16327 factor:1 | 1 (-0.28839) | -1 | -1 |
| G: -6727.20729 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12992.75507 HOMO: -6.38651 LUMO: -0.61770 factor:1 | 1 (-1.18209) | -1 | -1 |
| G: -6727.20729 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12993.18063 HOMO: -6.34297 LUMO: -0.33198 factor:1 | 1 (-1.60765) | -1 | -1 |
| G: -6727.20729 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12993.27916 HOMO: -7.51578 LUMO: 0.02177 factor:1 | 1 (-1.70618) | 1 | 1 |
| G: -6727.20729 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12993.12836 HOMO: -6.47359 LUMO: -0.22585 factor:1 | 1 (-1.55538) | -1 | -1 |
| G: -6727.20729 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12991.14900 HOMO: -6.68040 LUMO: -0.47076 factor:1 | -1 (0.42398) | -1 | -1 |
| G: -6727.20729 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12993.09715 HOMO: -6.75659 LUMO: -0.57688 factor:1 | 1 (-1.52416) | -1 | -1 |
| G: -6727.20729 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12993.17005 HOMO: -6.73754 LUMO: -0.61226 factor:1 | 1 (-1.59706) | -1 | -1 |
| G: -6727.20729 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12993.44227 HOMO: -7.37429 LUMO: 0.31293 factor:1 | 1 (-1.86929) | 1 | 1 |
| G: -6727.20729 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12993.27769 HOMO: -6.23413 LUMO: -0.90886 factor:1 | 1 (-1.70471) | -1 | -1 |
| G: -6727.20729 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12993.41508 HOMO: -6.51985 LUMO: -0.68028 factor:1 | 1 (-1.84210) | -1 | -1 |
| G: -6727.20729 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12993.06185 HOMO: -6.52257 LUMO: -0.77280 factor:1 | 1 (-1.48887) | -1 | -1 |
| G: -6727.20729 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12993.03415 HOMO: -7.29537 LUMO: 0.31837 factor:1 | 1 (-1.46117) | 1 | 1 |
| G: -6727.20729 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12993.13391 HOMO: -6.08447 LUMO: 0.25851 factor:1 | 1 (-1.56093) | -1 | -1 |
| G: -6727.20729 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12990.99431 HOMO: -6.20964 LUMO: 0.13606 factor:1 | -1 (0.57868) | -1 | -1 |
| G: -6727.20729 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12992.84332 HOMO: -6.49808 LUMO: -0.14150 factor:1 | 1 (-1.27034) | -1 | -1 |
| G: -6727.20729 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12992.05378 HOMO: -7.10761 LUMO: 0.28028 factor:1 | 1 (-0.48080) | 1 | 1 |
| G: -6727.20729 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12990.96519 HOMO: -6.60965 LUMO: -0.62858 factor:1 | -1 (0.60779) | -1 | -1 |
| G: -6727.20729 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12991.02495 HOMO: -6.40012 LUMO: -0.26939 factor:1 | -1 (0.54804) | -1 | -1 |
| G: -6727.20729 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12993.10591 HOMO: -6.65318 LUMO: -0.73199 factor:1 | 1 (-1.53293) | -1 | -1 |
| G: -6727.20729 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12992.31594 HOMO: -6.51441 LUMO: -0.44899 factor:1 | 1 (-0.74295) | -1 | -1 |
| G: -6727.20729 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12993.09015 HOMO: -6.28583 LUMO: -0.48708 factor:1 | 1 (-1.51717) | -1 | -1 |
| G: -6727.20729 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12993.05407 HOMO: -6.96884 LUMO: 0.19864 factor:1 | 1 (-1.48109) | -1 | -1 |
| G: -6727.20729 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12993.55144 HOMO: -6.89809 LUMO: 0.34558 factor:1 | 1 (-1.97846) | -1 | -1 |
| G: -6727.20729 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12992.24491 HOMO: -6.67495 LUMO: -0.15510 factor:1 | 1 (-0.67193) | -1 | -1 |
| G: -6727.20729 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12992.36192 HOMO: -7.34980 LUMO: 0.19864 factor:1 | 1 (-0.78894) | 1 | 1 |
| G: -6727.20729 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12993.44853 HOMO: -6.71305 LUMO: -0.81634 factor:1 | 1 (-1.87554) | -1 | -1 |
| G: -6727.20729 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12992.65480 HOMO: -6.39468 LUMO: -0.47076 factor:1 | 1 (-1.08182) | -1 | -1 |
| G: -6727.20729 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12992.41920 HOMO: -6.31304 LUMO: 1.39594 factor:1 | 1 (-0.84622) | -1 | -1 |
| G: -6727.20729 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12993.13551 HOMO: -6.57155 LUMO: 1.55105 factor:1 | 1 (-1.56253) | -1 | -1 |
| G: -6727.20729 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12993.06996 HOMO: -6.68312 LUMO: 1.69255 factor:1 | 1 (-1.49698) | -1 | -1 |
| G: -6727.20729 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12993.50573 HOMO: -6.61509 LUMO: 1.73881 factor:1 | 1 (-1.93274) | -1 | -1 |
| G: -6727.20729 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12992.97772 HOMO: -6.17971 LUMO: 1.90208 factor:1 | 1 (-1.40473) | -1 | -1 |
| G: -6727.20729 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12992.87782 HOMO: -6.53073 LUMO: 1.73337 factor:1 | 1 (-1.30484) | -1 | -1 |
| G: -6727.20729 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12993.63122 HOMO: -5.91303 LUMO: 1.90480 factor:1 | 1 (-2.05824) | -1 | -1 |
| G: -6727.20729 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12993.33084 HOMO: -6.42733 LUMO: 1.80139 factor:1 | 1 (-1.75786) | -1 | -1 |
| G: -6727.20729 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12993.17998 HOMO: -6.78924 LUMO: 2.31569 factor:1 | 1 (-1.60700) | -1 | -1 |
| G: -6727.20729 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12993.17105 HOMO: -6.04093 LUMO: 1.91568 factor:1 | 1 (-1.59807) | -1 | -1 |
| G: -6727.20729 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12990.46842 HOMO: -6.90081 LUMO: 2.36739 factor:1 | -1 (1.10456) | -1 | -1 |
| G: -6727.20729 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12991.77124 HOMO: -6.60965 LUMO: 2.18507 factor:1 | 1 (-0.19826) | -1 | -1 |
| G: -6727.20729 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12992.74949 HOMO: -6.75387 LUMO: 2.48712 factor:1 | 1 (-1.17651) | -1 | -1 |
| G: -6727.20729 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12991.97919 HOMO: -6.56883 LUMO: 1.71432 factor:1 | 1 (-0.40621) | -1 | -1 |
| G: -6727.20729 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12992.92392 HOMO: -6.41644 LUMO: 1.72792 factor:1 | 1 (-1.35094) | -1 | -1 |
| G: -6727.20729 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12992.77167 HOMO: -6.92530 LUMO: 2.54426 factor:1 | 1 (-1.19869) | -1 | -1 |
| G: -6727.20729 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12992.54832 HOMO: -6.41644 LUMO: 2.70209 factor:1 | 1 (-0.97534) | -1 | -1 |
| G: -6727.20729 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12992.08268 HOMO: -6.29671 LUMO: 2.14698 factor:1 | 1 (-0.50970) | -1 | -1 |
| G: -6727.20729 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12991.77650 HOMO: -6.29127 LUMO: 1.87486 factor:1 | 1 (-0.20351) | -1 | -1 |
| G: -6727.20729 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12992.49330 HOMO: -6.75931 LUMO: 2.78917 factor:1 | 1 (-0.92032) | -1 | -1 |
| G: -6727.20729 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12992.24053 HOMO: -6.40828 LUMO: 1.86942 factor:1 | 1 (-0.66755) | -1 | -1 |
| G: -6727.20729 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12993.12762 HOMO: -6.45726 LUMO: 1.97010 factor:1 | 1 (-1.55464) | -1 | -1 |
| G: -6727.20729 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12993.64965 HOMO: -6.43277 LUMO: 1.22723 factor:1 | 1 (-2.07666) | -1 | -1 |
| G: -6727.20729 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12993.01551 HOMO: -6.63414 LUMO: 1.62452 factor:1 | 1 (-1.44253) | -1 | -1 |
| G: -6727.20729 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12990.76614 HOMO: -6.54162 LUMO: 2.16058 factor:1 | -1 (0.80684) | -1 | -1 |
| G: -6727.20729 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12992.87834 HOMO: -6.40284 LUMO: 1.88575 factor:1 | 1 (-1.30536) | -1 | -1 |
| G: -6727.20729 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12993.01826 HOMO: -6.20964 LUMO: 1.84221 factor:1 | 1 (-1.44528) | -1 | -1 |
| G: -6727.20729 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12990.72959 HOMO: -6.58516 LUMO: 1.69799 factor:1 | -1 (0.84339) | -1 | -1 |
| G: -6727.20729 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12992.02241 HOMO: -6.44094 LUMO: 2.05446 factor:1 | 1 (-0.44942) | -1 | -1 |
| G: -6727.20729 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12992.57039 HOMO: -6.61509 LUMO: 2.16058 factor:1 | 1 (-0.99741) | -1 | -1 |
| G: -6727.20729 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12991.61799 HOMO: -6.65591 LUMO: 1.69527 factor:1 | 1 (-0.04501) | -1 | -1 |
| G: -6727.20729 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12992.67488 HOMO: -5.55112 LUMO: 1.80411 factor:1 | 1 (-1.10190) | -1 | -1 |
| G: -6727.20729 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12991.78284 HOMO: -6.68312 LUMO: 2.38100 factor:1 | 1 (-0.20985) | -1 | -1 |
| G: -6727.20729 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12992.97494 HOMO: -6.51168 LUMO: 2.14698 factor:1 | 1 (-1.40196) | -1 | -1 |
| G: -6727.20729 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12992.06281 HOMO: -6.04637 LUMO: 1.48302 factor:1 | 1 (-0.48983) | -1 | -1 |
| G: -6727.20729 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12990.93988 HOMO: -6.81645 LUMO: -0.74287 factor:1 | -1 (0.63310) | -1 | -1 |
| G: -6727.20729 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12991.76104 HOMO: -6.96884 LUMO: -0.97961 factor:1 | 1 (-0.18806) | -1 | -1 |
| G: -6727.20729 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12991.88801 HOMO: -6.45998 LUMO: 0.09796 factor:1 | 1 (-0.31503) | -1 | -1 |
| G: -6727.20729 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12993.23443 HOMO: -6.44638 LUMO: 0.09524 factor:1 | 1 (-1.66145) | -1 | -1 |
| G: -6727.20729 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12992.35153 HOMO: -6.16338 LUMO: -0.54151 factor:1 | 1 (-0.77854) | -1 | -1 |
| G: -6727.20729 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12993.11356 HOMO: -6.35930 LUMO: -0.47892 factor:1 | 1 (-1.54057) | -1 | -1 |
| G: -6727.20729 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12993.20670 HOMO: -6.65318 LUMO: -0.00272 factor:1 | 1 (-1.63372) | -1 | -1 |
| G: -6727.20729 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12993.31106 HOMO: -6.50080 LUMO: 0.14694 factor:1 | 1 (-1.73807) | -1 | -1 |
| G: -6727.20729 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12993.33119 HOMO: -6.60420 LUMO: 0.94968 factor:1 | 1 (-1.75821) | -1 | -1 |
| G: -6727.20729 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12993.19456 HOMO: -6.60148 LUMO: -0.77552 factor:1 | 1 (-1.62158) | -1 | -1 |
| G: -6727.20729 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12993.02313 HOMO: -6.81645 LUMO: -1.05580 factor:1 | 1 (-1.45015) | -1 | -1 |
| G: -6727.20729 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12993.10030 HOMO: -6.57971 LUMO: -0.82178 factor:1 | 1 (-1.52732) | -1 | -1 |
| G: -6727.20729 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12992.79978 HOMO: -6.09263 LUMO: -0.45171 factor:1 | 1 (-1.22680) | -1 | -1 |
| G: -6727.20729 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12993.03954 HOMO: -6.74298 LUMO: -0.61770 factor:1 | 1 (-1.46656) | -1 | -1 |
| G: -6727.20729 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12992.93401 HOMO: -6.72393 LUMO: 1.21091 factor:1 | 1 (-1.36103) | -1 | -1 |
| G: -6727.20729 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12992.31057 HOMO: -6.30488 LUMO: 1.70071 factor:1 | 1 (-0.73759) | -1 | -1 |
| G: -6727.20729 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12992.81848 HOMO: -6.38107 LUMO: 1.55649 factor:1 | 1 (-1.24549) | -1 | -1 |
| G: -6727.20729 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12993.14000 HOMO: -6.17154 LUMO: 1.46669 factor:1 | 1 (-1.56702) | -1 | -1 |
| G: -6727.20729 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12992.60623 HOMO: -6.86543 LUMO: 1.98643 factor:1 | 1 (-1.03324) | -1 | -1 |
| G: -6727.20729 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12991.90210 HOMO: -6.69944 LUMO: 1.65173 factor:1 | 1 (-0.32912) | -1 | -1 |
| G: -6727.20729 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12993.60796 HOMO: -6.77836 LUMO: 2.16331 factor:1 | 1 (-2.03498) | -1 | -1 |
| G: -6727.20729 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12992.70206 HOMO: -6.42189 LUMO: 2.36467 factor:1 | 1 (-1.12908) | -1 | -1 |
| G: -6727.20729 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12993.02501 HOMO: -7.00965 LUMO: 2.04358 factor:1 | 1 (-1.45203) | -1 | -1 |
| G: -6727.20729 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12993.36831 HOMO: -6.36746 LUMO: 2.13881 factor:1 | 1 (-1.79533) | -1 | -1 |
| G: -6727.20729 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12993.01083 HOMO: -6.37835 LUMO: 1.89935 factor:1 | 1 (-1.43785) | -1 | -1 |
| G: -6727.20729 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12993.01415 HOMO: -7.03959 LUMO: 1.27349 factor:1 | 1 (-1.44117) | -1 | -1 |
| G: -6727.20729 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12993.11132 HOMO: -6.67495 LUMO: -0.89253 factor:1 | 1 (-1.53834) | -1 | -1 |
| G: -6727.20729 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12993.13007 HOMO: -6.71849 LUMO: -0.97961 factor:1 | 1 (-1.55709) | -1 | -1 |
| G: -6727.20729 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12993.36570 HOMO: -6.47903 LUMO: 0.01633 factor:1 | 1 (-1.79271) | -1 | -1 |
| G: -6727.20729 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12992.65610 HOMO: -6.38379 LUMO: 0.01088 factor:1 | 1 (-1.08312) | -1 | -1 |
| G: -6727.20729 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12991.70724 HOMO: -6.49536 LUMO: -0.55239 factor:1 | 1 (-0.13426) | -1 | -1 |
| G: -6727.20729 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12992.78435 HOMO: -6.53345 LUMO: -0.53879 factor:1 | 1 (-1.21137) | -1 | -1 |
| G: -6727.20729 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12991.81720 HOMO: -6.16610 LUMO: 2.15514 factor:1 | 1 (-0.24422) | -1 | -1 |
| G: -6727.20729 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12993.11312 HOMO: -6.35114 LUMO: 1.98643 factor:1 | 1 (-1.54014) | -1 | -1 |
| G: -6727.20729 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12991.24718 HOMO: -6.43277 LUMO: 2.16058 factor:1 | -1 (0.32580) | -1 | -1 |
| G: -6727.20729 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12993.01821 HOMO: -6.89809 LUMO: 2.20684 factor:1 | 1 (-1.44522) | -1 | -1 |
| G: -6727.20729 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12992.96876 HOMO: -6.54434 LUMO: 1.93473 factor:1 | 1 (-1.39578) | -1 | -1 |
| G: -6727.20729 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12992.69676 HOMO: -6.72938 LUMO: 2.03269 factor:1 | 1 (-1.12378) | -1 | -1 |
| G: -6727.20729 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12993.08792 HOMO: -6.90353 LUMO: 2.19868 factor:1 | 1 (-1.51494) | -1 | -1 |
| G: -6727.20729 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12991.02799 HOMO: -6.41372 LUMO: 2.02453 factor:1 | -1 (0.54499) | -1 | -1 |
| G: -6727.20729 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12992.87445 HOMO: -6.46543 LUMO: 1.90752 factor:1 | 1 (-1.30147) | -1 | -1 |
| G: -6727.20729 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12992.67115 HOMO: -6.55522 LUMO: 2.11977 factor:1 | 1 (-1.09817) | -1 | -1 |
| G: -6727.20729 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12992.87434 HOMO: -6.28855 LUMO: 2.02181 factor:1 | 1 (-1.30136) | -1 | -1 |
| G: -6727.20729 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12992.77603 HOMO: -6.45726 LUMO: 1.52112 factor:1 | 1 (-1.20304) | -1 | -1 |
| G: -6727.20729 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12992.49044 HOMO: -6.37291 LUMO: 2.11705 factor:1 | 1 (-0.91746) | -1 | -1 |
| G: -6727.20729 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12992.94536 HOMO: -6.88448 LUMO: 2.24494 factor:1 | 1 (-1.37238) | -1 | -1 |
| G: -6727.20729 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12993.10311 HOMO: -6.86271 LUMO: 2.41637 factor:1 | 1 (-1.53012) | -1 | -1 |
| G: -6727.20729 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12993.23467 HOMO: -6.69400 LUMO: 2.34562 factor:1 | 1 (-1.66169) | -1 | -1 |
| G: -6727.20729 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12992.62639 HOMO: -6.18243 LUMO: 2.53882 factor:1 | 1 (-1.05341) | -1 | -1 |
| G: -6727.20729 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12991.58721 HOMO: -6.61237 LUMO: 2.54154 factor:1 | 1 (-0.01423) | -1 | -1 |
| G: -6727.20729 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12992.68854 HOMO: -6.69672 LUMO: 2.16331 factor:1 | 1 (-1.11556) | -1 | -1 |
| G: -6727.20729 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12991.88932 HOMO: -6.33481 LUMO: 2.34018 factor:1 | 1 (-0.31633) | -1 | -1 |
| G: -6727.20729 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12992.61099 HOMO: -5.99739 LUMO: 2.37283 factor:1 | 1 (-1.03801) | -1 | -1 |
| G: -6727.20729 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12991.88948 HOMO: -6.49808 LUMO: 2.47351 factor:1 | 1 (-0.31650) | -1 | -1 |
| G: -6727.20729 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12993.00833 HOMO: -6.22052 LUMO: 1.86398 factor:1 | 1 (-1.43535) | -1 | -1 |
| G: -6727.20729 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12993.15592 HOMO: -6.32665 LUMO: 2.28031 factor:1 | 1 (-1.58294) | -1 | -1 |
| G: -6727.20729 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12993.22126 HOMO: -5.98378 LUMO: 2.16331 factor:1 | 1 (-1.64828) | -1 | -1 |
| G: -6727.20729 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12993.50766 HOMO: -6.08991 LUMO: 2.30208 factor:1 | 1 (-1.93468) | -1 | -1 |
| G: -6727.20729 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12993.51830 HOMO: -7.07224 LUMO: 1.55105 factor:1 | 1 (-1.94531) | 1 | 1 |
| G: -6727.20729 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12992.71777 HOMO: -6.84638 LUMO: 1.76874 factor:1 | 1 (-1.14478) | -1 | -1 |
| G: -6727.20729 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12992.66895 HOMO: -6.68856 LUMO: 1.47758 factor:1 | 1 (-1.09597) | -1 | -1 |
| G: -6727.20729 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12992.93927 HOMO: -6.69672 LUMO: 1.71976 factor:1 | 1 (-1.36628) | -1 | -1 |
| G: -6727.20729 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12992.96441 HOMO: -6.86543 LUMO: 2.24766 factor:1 | 1 (-1.39143) | -1 | -1 |
| G: -6727.20729 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12993.05720 HOMO: -7.21646 LUMO: 1.71976 factor:1 | 1 (-1.48422) | 1 | 1 |
| G: -6727.20729 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12992.96289 HOMO: -6.94162 LUMO: 2.21773 factor:1 | 1 (-1.38990) | -1 | -1 |
| G: -6727.20729 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12993.13761 HOMO: -6.34842 LUMO: 2.04358 factor:1 | 1 (-1.56463) | -1 | -1 |
| G: -6727.20729 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12993.08324 HOMO: -6.53345 LUMO: 1.96738 factor:1 | 1 (-1.51026) | -1 | -1 |
| G: -6727.20729 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12993.07402 HOMO: -6.34842 LUMO: 1.88303 factor:1 | 1 (-1.50103) | -1 | -1 |
| G: -6727.20729 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12993.14670 HOMO: -6.38651 LUMO: 2.08983 factor:1 | 1 (-1.57372) | -1 | -1 |
| G: -6727.20729 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12992.95418 HOMO: -6.01372 LUMO: 1.43676 factor:1 | 1 (-1.38120) | -1 | -1 |
| G: -6727.20729 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12992.95040 HOMO: -6.30216 LUMO: 1.41771 factor:1 | 1 (-1.37741) | -1 | -1 |
| G: -6727.20729 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12993.12912 HOMO: -6.52801 LUMO: 1.77146 factor:1 | 1 (-1.55614) | -1 | -1 |
| G: -6727.20729 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12993.10234 HOMO: -6.53617 LUMO: 1.72792 factor:1 | 1 (-1.52936) | -1 | -1 |
| G: -6727.20729 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12993.22684 HOMO: -6.56611 LUMO: 2.20412 factor:1 | 1 (-1.65385) | -1 | -1 |
| G: -6727.20729 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12991.83342 HOMO: -6.66679 LUMO: -0.72927 factor:1 | 1 (-0.26044) | -1 | -1 |
| G: -6727.20729 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12992.73692 HOMO: -6.85455 LUMO: -0.85444 factor:1 | 1 (-1.16394) | -1 | -1 |
| G: -6727.20729 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12993.36311 HOMO: -7.21646 LUMO: 0.27211 factor:1 | 1 (-1.79013) | 1 | 1 |
| G: -6727.20729 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12993.15456 HOMO: -6.57971 LUMO: -0.41361 factor:1 | 1 (-1.58158) | -1 | -1 |
| G: -6727.20729 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12991.96494 HOMO: -7.03142 LUMO: -1.14288 factor:1 | 1 (-0.39195) | -1 | -1 |
| G: -6727.20729 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12992.24483 HOMO: -6.29944 LUMO: 0.06803 factor:1 | 1 (-0.67185) | -1 | -1 |
| G: -6727.20729 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12992.74364 HOMO: -6.47359 LUMO: 0.28028 factor:1 | 1 (-1.17066) | -1 | -1 |
| G: -6727.20729 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12993.31473 HOMO: -6.42189 LUMO: 1.61364 factor:1 | 1 (-1.74175) | -1 | -1 |
| G: -6727.20729 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12992.81997 HOMO: -6.41100 LUMO: 1.80956 factor:1 | 1 (-1.24699) | -1 | -1 |
| G: -6727.20729 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12993.18172 HOMO: -6.83278 LUMO: 1.83949 factor:1 | 1 (-1.60874) | -1 | -1 |
| G: -6727.20729 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12991.93666 HOMO: -6.78380 LUMO: -0.76192 factor:1 | 1 (-0.36368) | -1 | -1 |
| G: -6727.20729 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12992.02654 HOMO: -6.95795 LUMO: 2.13609 factor:1 | 1 (-0.45356) | -1 | -1 |
| G: -6727.20729 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12992.69602 HOMO: -6.57155 LUMO: 1.89119 factor:1 | 1 (-1.12304) | -1 | -1 |
| G: -6727.20729 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12992.91317 HOMO: -6.65591 LUMO: 1.93745 factor:1 | 1 (-1.34019) | -1 | -1 |
| G: -6727.20729 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12992.66057 HOMO: -6.44638 LUMO: 2.26943 factor:1 | 1 (-1.08758) | -1 | -1 |
| G: -6727.20729 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12992.14464 HOMO: -5.88038 LUMO: 1.90480 factor:1 | 1 (-0.57166) | -1 | -1 |
| G: -6727.20729 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12993.40747 HOMO: -6.22052 LUMO: 2.17691 factor:1 | 1 (-1.83448) | -1 | -1 |
| G: -6727.20729 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12992.72620 HOMO: -6.04637 LUMO: 2.23950 factor:1 | 1 (-1.15322) | -1 | -1 |
| G: -6727.20729 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12993.27057 HOMO: -6.44366 LUMO: 2.24766 factor:1 | 1 (-1.69758) | -1 | -1 |
| G: -6727.20729 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12992.74313 HOMO: -6.81917 LUMO: 2.08439 factor:1 | 1 (-1.17014) | -1 | -1 |
| G: -6727.20729 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12992.51137 HOMO: -6.48447 LUMO: 2.28576 factor:1 | 1 (-0.93838) | -1 | -1 |
| G: -6727.20729 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12992.96044 HOMO: -6.54434 LUMO: 1.99187 factor:1 | 1 (-1.38745) | -1 | -1 |
| G: -6727.20729 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12992.61692 HOMO: -6.17698 LUMO: -0.65852 factor:1 | 1 (-1.04394) | -1 | -1 |
| G: -6727.20729 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12993.48921 HOMO: -6.08174 LUMO: -0.58504 factor:1 | 1 (-1.91623) | -1 | -1 |
| G: -6727.20729 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12992.50769 HOMO: -6.55250 LUMO: -0.86804 factor:1 | 1 (-0.93471) | -1 | -1 |
| G: -6727.20729 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12990.37307 HOMO: -6.57699 LUMO: -0.89525 factor:1 | -1 (1.19991) | -1 | -1 |
| G: -6727.20729 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12992.87396 HOMO: -6.63141 LUMO: -1.04220 factor:1 | 1 (-1.30098) | -1 | -1 |
| G: -6727.20729 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12992.96670 HOMO: -6.69128 LUMO: -0.76736 factor:1 | 1 (-1.39371) | -1 | -1 |
| G: -6727.20729 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12992.62146 HOMO: -6.25318 LUMO: -1.03131 factor:1 | 1 (-1.04848) | -1 | -1 |
| G: -6727.20729 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12991.69704 HOMO: -6.69944 LUMO: 0.01905 factor:1 | 1 (-0.12406) | -1 | -1 |
| G: -6727.80684 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12991.26024 HOMO: -6.28583 LUMO: 0.38368 factor:1 | -1 (0.91229) | -1 | -1 |
| G: -6727.80684 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12991.00976 HOMO: -6.90081 LUMO: -0.83811 factor:1 | -1 (1.16277) | -1 | -1 |
| G: -6727.80684 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12991.13880 HOMO: -6.78380 LUMO: -0.10068 factor:1 | -1 (1.03373) | -1 | -1 |
| G: -6727.80684 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12990.82383 HOMO: -6.30488 LUMO: -0.98505 factor:1 | -1 (1.34871) | -1 | -1 |
| G: -6727.80684 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12990.59914 HOMO: -6.29671 LUMO: -1.79051 factor:1 | -1 (1.57339) | -1 | -1 |
| G: -6727.80684 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12990.85749 HOMO: -6.76747 LUMO: -0.22041 factor:1 | -1 (1.31504) | -1 | -1 |
| G: -6727.80684 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12990.88976 HOMO: -6.22597 LUMO: -0.94968 factor:1 | -1 (1.28277) | -1 | -1 |
| G: -6727.80684 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12990.95806 HOMO: -6.73482 LUMO: 0.05987 factor:1 | -1 (1.21447) | -1 | -1 |
| G: -6727.80684 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12990.85215 HOMO: -6.28855 LUMO: 0.34831 factor:1 | -1 (1.32038) | -1 | -1 |
| G: -6727.80684 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12991.17102 HOMO: -6.69400 LUMO: 0.25307 factor:1 | -1 (1.00152) | -1 | -1 |
| G: -6727.80684 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12990.83561 HOMO: -6.70216 LUMO: 0.61226 factor:1 | -1 (1.33692) | -1 | -1 |
| G: -6727.80684 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12991.02775 HOMO: -6.70216 LUMO: 0.17415 factor:1 | -1 (1.14478) | -1 | -1 |
| G: -6727.80684 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12990.63471 HOMO: -6.70761 LUMO: 0.24762 factor:1 | -1 (1.53782) | -1 | -1 |
| G: -6727.80684 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12990.80219 HOMO: -6.68856 LUMO: -0.84900 factor:1 | -1 (1.37034) | -1 | -1 |
| G: -6727.80684 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12990.98786 HOMO: -6.71033 LUMO: -0.38640 factor:1 | -1 (1.18467) | -1 | -1 |
| G: -6727.80684 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12990.84347 HOMO: -6.24501 LUMO: -0.09252 factor:1 | -1 (1.32906) | -1 | -1 |
| G: -6727.80684 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12993.82026 HOMO: -6.81645 LUMO: -0.07347 factor:1 | 1 (-1.64773) | -1 | -1 |
| G: -6727.80684 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12993.33114 HOMO: -6.49536 LUMO: 0.09796 factor:1 | 1 (-1.15861) | -1 | -1 |
| G: -6727.80684 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12993.38417 HOMO: -6.71033 LUMO: -0.26395 factor:1 | 1 (-1.21164) | -1 | -1 |
| G: -6727.80684 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12993.53280 HOMO: -6.70489 LUMO: -0.09252 factor:1 | 1 (-1.36027) | -1 | -1 |
| G: -6727.80684 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12993.40551 HOMO: -6.23685 LUMO: 0.39729 factor:1 | 1 (-1.23298) | -1 | -1 |
| G: -6727.80684 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12993.41383 HOMO: -6.69400 LUMO: -0.05442 factor:1 | 1 (-1.24130) | -1 | -1 |
| G: -6727.80684 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12993.43702 HOMO: -6.36202 LUMO: 0.09796 factor:1 | 1 (-1.26449) | -1 | -1 |
| G: -6727.80684 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12993.32866 HOMO: -6.54978 LUMO: 0.15510 factor:1 | 1 (-1.15613) | -1 | -1 |
| G: -6727.80684 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12993.79060 HOMO: -6.77836 LUMO: 0.25851 factor:1 | 1 (-1.61807) | -1 | -1 |
| G: -6727.80684 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12993.27301 HOMO: -5.70623 LUMO: 0.73471 factor:1 | 1 (-1.10048) | -1 | -1 |
| G: -6727.80684 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12993.24926 HOMO: -5.58378 LUMO: 0.89253 factor:1 | 1 (-1.07673) | -1 | -1 |
| G: -6727.80684 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12992.94465 HOMO: -5.68718 LUMO: 0.87893 factor:1 | 1 (-0.77212) | -1 | -1 |
| G: -6727.80684 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12992.08826 HOMO: -5.10486 LUMO: 1.11567 factor:1 | -1 (0.08427) | -1 | -1 |
| G: -6727.80684 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12993.43424 HOMO: -4.59328 LUMO: 1.27621 factor:1 | 1 (-1.26171) | -1 | -1 |
| G: -6727.80684 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12993.31723 HOMO: -4.45450 LUMO: 1.82044 factor:1 | 1 (-1.14470) | -1 | -1 |
| G: -6727.80684 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12993.41081 HOMO: -4.64226 LUMO: 1.70615 factor:1 | 1 (-1.23828) | -1 | -1 |
| G: -6727.80684 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12992.00246 HOMO: -5.04227 LUMO: 1.04492 factor:1 | -1 (0.17007) | -1 | -1 |
| G: -6727.80684 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12992.89241 HOMO: -4.85723 LUMO: 0.93607 factor:1 | 1 (-0.71988) | -1 | -1 |
| G: -6727.80684 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12993.66072 HOMO: -4.72934 LUMO: 1.00410 factor:1 | 1 (-1.48819) | -1 | -1 |
| G: -6727.80684 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12993.11024 HOMO: -4.56335 LUMO: 1.56738 factor:1 | 1 (-0.93770) | -1 | -1 |
| G: -6727.80684 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12992.98642 HOMO: -5.48854 LUMO: 0.33198 factor:1 | 1 (-0.81389) | -1 | -1 |
| G: -6727.80684 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12993.20817 HOMO: -4.97424 LUMO: 1.33608 factor:1 | 1 (-1.03564) | -1 | -1 |
| G: -6727.80684 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12992.98593 HOMO: -4.60145 LUMO: 1.74697 factor:1 | 1 (-0.81340) | -1 | -1 |
| G: -6727.80684 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12993.19535 HOMO: -5.60010 LUMO: 0.74831 factor:1 | 1 (-1.02282) | -1 | -1 |
| G: -6727.80684 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12993.06724 HOMO: -5.66541 LUMO: 0.66668 factor:1 | 1 (-0.89471) | -1 | -1 |
| G: -6727.80684 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12993.17954 HOMO: -6.50080 LUMO: 0.07075 factor:1 | 1 (-1.00701) | -1 | -1 |
| G: -6727.80684 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12993.11247 HOMO: -5.79603 LUMO: 0.22313 factor:1 | 1 (-0.93994) | -1 | -1 |
| G: -6727.80684 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12993.62935 HOMO: -4.68036 LUMO: 1.29798 factor:1 | 1 (-1.45682) | -1 | -1 |
| G: -6727.80684 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12993.54472 HOMO: -4.84363 LUMO: 1.34424 factor:1 | 1 (-1.37219) | -1 | -1 |
| G: -6727.80684 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12993.28327 HOMO: -4.62321 LUMO: 1.82861 factor:1 | 1 (-1.11074) | -1 | -1 |
| G: -6727.80684 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12993.34336 HOMO: -5.83684 LUMO: 0.82178 factor:1 | 1 (-1.17082) | -1 | -1 |
| G: -6727.80684 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12993.11285 HOMO: -5.27629 LUMO: 0.57960 factor:1 | 1 (-0.94032) | -1 | -1 |
| G: -6727.80684 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12992.65706 HOMO: -5.15928 LUMO: -2.96876 factor:1 | 1 (-0.48453) | -1 | -1 |
| G: -6727.80684 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12993.11690 HOMO: -5.08853 LUMO: 0.89253 factor:1 | 1 (-0.94437) | -1 | -1 |
| G: -6727.80684 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12993.00585 HOMO: -6.42461 LUMO: 0.04354 factor:1 | 1 (-0.83332) | -1 | -1 |
| G: -6727.80684 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12993.00974 HOMO: -6.42733 LUMO: -0.00544 factor:1 | 1 (-0.83721) | -1 | -1 |
| G: -6727.80684 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12993.59245 HOMO: -5.87494 LUMO: 0.69933 factor:1 | 1 (-1.41992) | -1 | -1 |
| G: -6727.80684 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12993.29840 HOMO: -5.07492 LUMO: 1.02587 factor:1 | 1 (-1.12587) | -1 | -1 |
| G: -6727.80684 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12993.36477 HOMO: -4.44362 LUMO: 1.99187 factor:1 | 1 (-1.19224) | -1 | -1 |
| G: -6727.80684 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12993.29187 HOMO: -5.82052 LUMO: 0.43810 factor:1 | 1 (-1.11934) | -1 | -1 |
| G: -6727.80684 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12992.96313 HOMO: -5.75793 LUMO: 0.76464 factor:1 | 1 (-0.79060) | -1 | -1 |
| G: -6727.80684 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12992.07743 HOMO: -5.09669 LUMO: 0.72382 factor:1 | -1 (0.09510) | -1 | -1 |
| G: -6727.80684 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12993.25622 HOMO: -6.75387 LUMO: -2.02453 factor:1 | 1 (-1.08369) | -1 | -1 |
| G: -6727.80684 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12993.07021 HOMO: -5.02322 LUMO: 1.14832 factor:1 | 1 (-0.89768) | -1 | -1 |
| G: -6727.80684 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12993.29606 HOMO: -5.75521 LUMO: 0.73471 factor:1 | 1 (-1.12353) | -1 | -1 |
| G: -6727.80684 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12993.26376 HOMO: -5.89943 LUMO: 0.54967 factor:1 | 1 (-1.09123) | -1 | -1 |
| G: -6727.80684 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12993.29799 HOMO: -5.80147 LUMO: 0.72382 factor:1 | 1 (-1.12546) | -1 | -1 |
| G: -6727.80684 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12992.99954 HOMO: -6.16066 LUMO: 0.39457 factor:1 | 1 (-0.82701) | -1 | -1 |
| G: -6727.80684 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12993.00226 HOMO: -5.98650 LUMO: 0.76736 factor:1 | 1 (-0.82973) | -1 | -1 |
| G: -6727.80684 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12992.84193 HOMO: -4.74839 LUMO: 1.88847 factor:1 | 1 (-0.66940) | -1 | -1 |
| G: -6727.80684 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12991.03578 HOMO: -5.62459 LUMO: 0.26939 factor:1 | -1 (1.13676) | -1 | -1 |
| G: -6727.80684 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12992.69330 HOMO: -4.88172 LUMO: 1.30070 factor:1 | 1 (-0.52077) | -1 | -1 |
| G: -6727.80684 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12991.86137 HOMO: -5.09397 LUMO: 0.98505 factor:1 | -1 (0.31116) | -1 | -1 |
| G: -6727.80684 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12992.75507 HOMO: -6.50080 LUMO: -0.28300 factor:1 | 1 (-0.58254) | -1 | -1 |
| G: -6727.80684 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12993.18063 HOMO: -5.04227 LUMO: 1.49935 factor:1 | 1 (-1.00810) | -1 | -1 |
| G: -6727.80684 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12993.27916 HOMO: -5.22731 LUMO: 0.88437 factor:1 | 1 (-1.10663) | -1 | -1 |
| G: -6727.80684 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12993.12836 HOMO: -4.95519 LUMO: 1.25717 factor:1 | 1 (-0.95583) | -1 | -1 |
| G: -6727.80684 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12991.14900 HOMO: -4.61233 LUMO: 1.27621 factor:1 | -1 (1.02353) | -1 | -1 |
| G: -6727.80684 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12993.09715 HOMO: -4.70757 LUMO: 1.63813 factor:1 | 1 (-0.92462) | -1 | -1 |
| G: -6727.80684 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12993.17005 HOMO: -4.85179 LUMO: 1.11839 factor:1 | 1 (-0.99751) | -1 | -1 |
| G: -6727.80684 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12993.44227 HOMO: -4.97696 LUMO: 1.00138 factor:1 | 1 (-1.26974) | -1 | -1 |
| G: -6727.80684 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12993.27769 HOMO: -5.64636 LUMO: 0.81090 factor:1 | 1 (-1.10516) | -1 | -1 |
| G: -6727.80684 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12993.41508 HOMO: -4.37831 LUMO: 1.90208 factor:1 | 1 (-1.24255) | -1 | -1 |
| G: -6727.80684 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12993.06185 HOMO: -4.67764 LUMO: 1.54561 factor:1 | 1 (-0.88932) | -1 | -1 |
| G: -6727.80684 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12993.03415 HOMO: -5.87766 LUMO: 0.42994 factor:1 | 1 (-0.86162) | -1 | -1 |
| G: -6727.80684 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12993.13391 HOMO: -6.03821 LUMO: 0.32382 factor:1 | 1 (-0.96138) | -1 | -1 |
| G: -6727.80684 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12990.99431 HOMO: -5.99739 LUMO: 0.69389 factor:1 | -1 (1.17823) | -1 | -1 |
| G: -6727.80684 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12992.84332 HOMO: -6.43821 LUMO: 0.15238 factor:1 | 1 (-0.67079) | -1 | -1 |
| G: -6727.80684 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12992.05378 HOMO: -6.63414 LUMO: -0.07347 factor:1 | -1 (0.11875) | -1 | -1 |
| G: -6727.80684 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12990.96519 HOMO: -6.50080 LUMO: 0.10068 factor:1 | -1 (1.20734) | -1 | -1 |
| G: -6727.80684 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12991.02495 HOMO: -6.49264 LUMO: 0.19592 factor:1 | -1 (1.14759) | -1 | -1 |
| G: -6727.80684 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12993.10591 HOMO: -5.83956 LUMO: 0.12517 factor:1 | 1 (-0.93338) | -1 | -1 |
| G: -6727.80684 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12992.31594 HOMO: -6.50896 LUMO: 0.19048 factor:1 | 1 (-0.14340) | -1 | -1 |
| G: -6727.80684 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12993.09015 HOMO: -6.56611 LUMO: 0.04898 factor:1 | 1 (-0.91762) | -1 | -1 |
| G: -6727.80684 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12993.05407 HOMO: -6.68040 LUMO: -0.08436 factor:1 | 1 (-0.88154) | -1 | -1 |
| G: -6727.80684 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12993.55144 HOMO: -6.73754 LUMO: -0.08708 factor:1 | 1 (-1.37891) | -1 | -1 |
| G: -6727.80684 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12992.24491 HOMO: -6.80285 LUMO: -0.10612 factor:1 | 1 (-0.07238) | -1 | -1 |
| G: -6727.80684 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12992.36192 HOMO: -6.35658 LUMO: 0.02177 factor:1 | 1 (-0.18939) | -1 | -1 |
| G: -6727.80684 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12993.44853 HOMO: -5.74160 LUMO: 0.14694 factor:1 | 1 (-1.27600) | -1 | -1 |
| G: -6727.80684 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12992.65480 HOMO: -4.78376 LUMO: 0.92791 factor:1 | 1 (-0.48227) | -1 | -1 |
| G: -6727.80684 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12992.41920 HOMO: -5.90215 LUMO: 0.36463 factor:1 | 1 (-0.24667) | -1 | -1 |
| G: -6727.80684 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12993.13551 HOMO: -4.99329 LUMO: 0.85988 factor:1 | 1 (-0.96298) | -1 | -1 |
| G: -6727.80684 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12993.06996 HOMO: -4.93887 LUMO: 1.33608 factor:1 | 1 (-0.89743) | -1 | -1 |
| G: -6727.80684 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12993.50573 HOMO: -5.19193 LUMO: 0.50341 factor:1 | 1 (-1.33319) | -1 | -1 |
| G: -6727.80684 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12992.97772 HOMO: -6.64502 LUMO: -1.98643 factor:1 | 1 (-0.80518) | -1 | -1 |
| G: -6727.80684 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12992.87782 HOMO: -5.15384 LUMO: 0.94968 factor:1 | 1 (-0.70529) | -1 | -1 |
| G: -6727.80684 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12993.63122 HOMO: -6.31032 LUMO: 0.08436 factor:1 | 1 (-1.45869) | -1 | -1 |
| G: -6727.80684 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12993.33084 HOMO: -4.88716 LUMO: 0.82995 factor:1 | 1 (-1.15831) | -1 | -1 |
| G: -6727.80684 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12993.17998 HOMO: -5.57017 LUMO: 0.19320 factor:1 | 1 (-1.00745) | -1 | -1 |
| G: -6727.80684 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12993.17105 HOMO: -4.92254 LUMO: 0.93879 factor:1 | 1 (-0.99852) | -1 | -1 |
| G: -6727.80684 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12990.46842 HOMO: -4.77288 LUMO: 1.60003 factor:1 | -1 (1.70411) | -1 | -1 |
| G: -6727.80684 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12991.77124 HOMO: -4.97696 LUMO: 0.89798 factor:1 | -1 (0.40129) | -1 | -1 |
| G: -6727.80684 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12992.74949 HOMO: -5.00690 LUMO: 1.14288 factor:1 | 1 (-0.57696) | -1 | -1 |
| G: -6727.80684 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12991.97919 HOMO: -4.88444 LUMO: 1.48574 factor:1 | -1 (0.19334) | -1 | -1 |
| G: -6727.80684 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12992.92392 HOMO: -5.03955 LUMO: 1.51023 factor:1 | 1 (-0.75139) | -1 | -1 |
| G: -6727.80684 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12992.77167 HOMO: -5.22459 LUMO: 0.99049 factor:1 | 1 (-0.59914) | -1 | -1 |
| G: -6727.80684 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12992.54832 HOMO: -5.29534 LUMO: 0.96056 factor:1 | 1 (-0.37579) | -1 | -1 |
| G: -6727.80684 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12992.08268 HOMO: -5.35520 LUMO: 0.68301 factor:1 | -1 (0.08985) | -1 | -1 |
| G: -6727.80684 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12991.77650 HOMO: -5.27357 LUMO: 1.18642 factor:1 | -1 (0.39603) | -1 | -1 |
| G: -6727.80684 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12992.49330 HOMO: -5.79875 LUMO: 0.61770 factor:1 | 1 (-0.32077) | -1 | -1 |
| G: -6727.80684 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12992.24053 HOMO: -7.64640 LUMO: -2.45175 factor:1 | 1 (-0.06800) | -1 | -1 |
| G: -6727.80684 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12993.12762 HOMO: -7.46953 LUMO: -1.29798 factor:1 | 1 (-0.95509) | 1 | 1 |
| G: -6727.80684 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12993.64965 HOMO: -7.95389 LUMO: -0.37280 factor:1 | 1 (-1.47712) | 1 | 1 |
| G: -6727.80684 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12993.01551 HOMO: -7.23279 LUMO: -1.19186 factor:1 | 1 (-0.84298) | 1 | 1 |
| G: -6727.80684 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12990.76614 HOMO: -7.14299 LUMO: -1.12927 factor:1 | -1 (1.40639) | 1 | 1 |
| G: -6727.80684 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12992.87834 HOMO: -6.93074 LUMO: 0.31565 factor:1 | 1 (-0.70581) | -1 | -1 |
| G: -6727.80684 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12993.01826 HOMO: -6.63141 LUMO: 0.28028 factor:1 | 1 (-0.84573) | -1 | -1 |
| G: -6727.80684 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12990.72959 HOMO: -7.10489 LUMO: -1.07213 factor:1 | -1 (1.44294) | 1 | 1 |
| G: -6727.80684 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12992.02241 HOMO: -7.00693 LUMO: -0.69389 factor:1 | -1 (0.15013) | -1 | -1 |
| G: -6727.80684 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12992.57039 HOMO: -8.50356 LUMO: -1.79595 factor:1 | 1 (-0.39786) | -1 | -1 |
| G: -6727.80684 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12991.61799 HOMO: -7.79334 LUMO: -2.33746 factor:1 | -1 (0.55454) | -1 | -1 |
| G: -6727.80684 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12992.67488 HOMO: -7.24367 LUMO: -0.85172 factor:1 | 1 (-0.50235) | 1 | 1 |
| G: -6727.80684 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12991.78284 HOMO: -7.94028 LUMO: -0.20136 factor:1 | -1 (0.38969) | 1 | 1 |
| G: -6727.80684 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12992.97494 HOMO: -7.22462 LUMO: 0.84627 factor:1 | 1 (-0.80241) | 1 | 1 |
| G: -6727.80684 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12992.06281 HOMO: -6.54978 LUMO: 0.34831 factor:1 | -1 (0.10972) | -1 | -1 |
| G: -6727.80684 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12990.93988 HOMO: -6.86815 LUMO: 0.32109 factor:1 | -1 (1.23265) | -1 | -1 |
| G: -6727.80684 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12991.76104 HOMO: -7.17564 LUMO: -1.28438 factor:1 | -1 (0.41149) | 1 | 1 |
| G: -6727.80684 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12991.88801 HOMO: -7.03142 LUMO: -1.12655 factor:1 | -1 (0.28452) | -1 | -1 |
| G: -6727.80684 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12993.23443 HOMO: -7.39878 LUMO: 0.15783 factor:1 | 1 (-1.06190) | 1 | 1 |
| G: -6727.80684 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12992.35153 HOMO: -7.25728 LUMO: 0.42178 factor:1 | 1 (-0.17900) | 1 | 1 |
| G: -6727.80684 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12993.11356 HOMO: -6.86543 LUMO: 0.93879 factor:1 | 1 (-0.94102) | -1 | -1 |
| G: -6727.80684 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12993.20670 HOMO: -7.09673 LUMO: -0.69661 factor:1 | 1 (-1.03417) | 1 | 1 |
| G: -6727.80684 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12993.31106 HOMO: -7.74708 LUMO: 0.01088 factor:1 | 1 (-1.13852) | 1 | 1 |
| G: -6727.80684 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12993.33119 HOMO: -6.80557 LUMO: 0.46531 factor:1 | 1 (-1.15866) | -1 | -1 |
| G: -6727.80684 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12993.19456 HOMO: -7.29265 LUMO: 1.31975 factor:1 | 1 (-1.02203) | 1 | 1 |
| G: -6727.80684 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12993.02313 HOMO: -6.93618 LUMO: 0.29388 factor:1 | 1 (-0.85060) | -1 | -1 |
| G: -6727.80684 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12993.10030 HOMO: -6.53073 LUMO: 0.71022 factor:1 | 1 (-0.92777) | -1 | -1 |
| G: -6727.80684 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12992.79978 HOMO: -6.41917 LUMO: -1.24084 factor:1 | 1 (-0.62725) | -1 | -1 |
| G: -6727.80684 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12993.03954 HOMO: -6.67495 LUMO: -1.09118 factor:1 | 1 (-0.86701) | -1 | -1 |
| G: -6727.80684 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12992.93401 HOMO: -6.97156 LUMO: -0.53606 factor:1 | 1 (-0.76148) | -1 | -1 |
| G: -6727.80684 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12992.31057 HOMO: -6.85183 LUMO: -0.45715 factor:1 | 1 (-0.13804) | -1 | -1 |
| G: -6727.80684 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12992.81848 HOMO: -7.12666 LUMO: -0.67484 factor:1 | 1 (-0.64594) | 1 | 1 |
| G: -6727.80684 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12993.14000 HOMO: -7.49946 LUMO: -0.14694 factor:1 | 1 (-0.96747) | 1 | 1 |
| G: -6727.80684 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12992.60623 HOMO: -7.44231 LUMO: 0.58232 factor:1 | 1 (-0.43370) | 1 | 1 |
| G: -6727.80684 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12991.90210 HOMO: -7.36340 LUMO: -0.68301 factor:1 | -1 (0.27043) | 1 | 1 |
| G: -6727.80684 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12993.60796 HOMO: -6.13073 LUMO: -0.54967 factor:1 | 1 (-1.43543) | -1 | -1 |
| G: -6727.80684 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12992.70206 HOMO: -7.81511 LUMO: -0.06531 factor:1 | 1 (-0.52953) | 1 | 1 |
| G: -6727.80684 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12993.02501 HOMO: -7.26816 LUMO: -1.02587 factor:1 | 1 (-0.85248) | 1 | 1 |
| G: -6727.80684 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12993.36831 HOMO: -7.98110 LUMO: -0.17960 factor:1 | 1 (-1.19578) | 1 | 1 |
| G: -6727.80684 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12993.01083 HOMO: -7.44776 LUMO: -1.00954 factor:1 | 1 (-0.83830) | 1 | 1 |
| G: -6727.80684 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12993.01415 HOMO: -7.47769 LUMO: -1.02859 factor:1 | 1 (-0.84162) | 1 | 1 |
| G: -6727.80684 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12993.11132 HOMO: -6.75659 LUMO: 0.39457 factor:1 | 1 (-0.93879) | -1 | -1 |
| G: -6727.80684 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12993.13007 HOMO: -6.71849 LUMO: 0.36735 factor:1 | 1 (-0.95754) | -1 | -1 |
| G: -6727.80684 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12993.36570 HOMO: -7.64096 LUMO: -1.43948 factor:1 | 1 (-1.19316) | 1 | 1 |
| G: -6727.80684 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12992.65610 HOMO: -7.83144 LUMO: -1.36601 factor:1 | 1 (-0.48357) | 1 | 1 |
| G: -6727.80684 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12991.70724 HOMO: -7.19469 LUMO: 0.35103 factor:1 | -1 (0.46529) | 1 | 1 |
| G: -6727.80684 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12992.78435 HOMO: -7.03414 LUMO: 0.20409 factor:1 | 1 (-0.61182) | -1 | -1 |
| G: -6727.80684 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12991.81720 HOMO: -7.22734 LUMO: 0.31293 factor:1 | -1 (0.35533) | 1 | 1 |
| G: -6727.80684 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12993.11312 HOMO: -6.93618 LUMO: 0.56055 factor:1 | 1 (-0.94059) | -1 | -1 |
| G: -6727.80684 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12991.24718 HOMO: -6.94707 LUMO: -0.88709 factor:1 | -1 (0.92535) | -1 | -1 |
| G: -6727.80684 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12993.01821 HOMO: -6.86543 LUMO: -0.83267 factor:1 | 1 (-0.84568) | -1 | -1 |
| G: -6727.80684 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12992.96876 HOMO: -6.82189 LUMO: -1.15376 factor:1 | 1 (-0.79623) | -1 | -1 |
| G: -6727.80684 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12992.69676 HOMO: -6.65046 LUMO: -0.46531 factor:1 | 1 (-0.52423) | -1 | -1 |
| G: -6727.80684 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12993.08792 HOMO: -6.52529 LUMO: 0.20953 factor:1 | 1 (-0.91539) | -1 | -1 |
| G: -6727.80684 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12991.02799 HOMO: -6.80557 LUMO: 0.44355 factor:1 | -1 (1.14454) | -1 | -1 |
| G: -6727.80684 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12992.87445 HOMO: -6.93074 LUMO: -0.81634 factor:1 | 1 (-0.70192) | -1 | -1 |
| G: -6727.80684 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12992.67115 HOMO: -7.43143 LUMO: -0.45987 factor:1 | 1 (-0.49862) | 1 | 1 |
| G: -6727.80684 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12992.87434 HOMO: -7.07224 LUMO: -0.68028 factor:1 | 1 (-0.70181) | 1 | 1 |
| G: -6727.80684 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12992.77603 HOMO: -6.68040 LUMO: -0.71566 factor:1 | 1 (-0.60349) | -1 | -1 |
| G: -6727.80684 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12992.49044 HOMO: -6.26406 LUMO: -1.09934 factor:1 | 1 (-0.31791) | -1 | -1 |
| G: -6727.80684 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12992.94536 HOMO: -5.94569 LUMO: -0.72110 factor:1 | 1 (-0.77283) | -1 | -1 |
| G: -6727.80684 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12993.10311 HOMO: -6.12256 LUMO: -0.42178 factor:1 | 1 (-0.93057) | -1 | -1 |
| G: -6727.80684 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12993.23467 HOMO: -6.09807 LUMO: 0.11429 factor:1 | 1 (-1.06214) | -1 | -1 |
| G: -6727.80684 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12992.62639 HOMO: -7.35252 LUMO: -0.55783 factor:1 | 1 (-0.45386) | 1 | 1 |
| G: -6727.80684 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12991.58721 HOMO: -7.57837 LUMO: -0.76736 factor:1 | -1 (0.58532) | 1 | 1 |
| G: -6727.80684 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12992.68854 HOMO: -6.16066 LUMO: 0.01905 factor:1 | 1 (-0.51601) | -1 | -1 |
| G: -6727.80684 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12991.88932 HOMO: -6.13345 LUMO: -0.41906 factor:1 | -1 (0.28322) | -1 | -1 |
| G: -6727.80684 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12992.61099 HOMO: -6.10351 LUMO: -0.33742 factor:1 | 1 (-0.43846) | -1 | -1 |
| G: -6727.80684 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12991.88948 HOMO: -7.24639 LUMO: -0.51702 factor:1 | -1 (0.28305) | 1 | 1 |
| G: -6727.80684 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12993.00833 HOMO: -6.98244 LUMO: -1.82044 factor:1 | 1 (-0.83580) | -1 | -1 |
| G: -6727.80684 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12993.15592 HOMO: -6.37563 LUMO: -1.67622 factor:1 | 1 (-0.98339) | -1 | -1 |
| G: -6727.80684 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12993.22126 HOMO: -5.79058 LUMO: -2.55243 factor:1 | 1 (-1.04873) | -1 | -1 |
| G: -6727.80684 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12993.50766 HOMO: -6.34025 LUMO: -0.27483 factor:1 | 1 (-1.33513) | -1 | -1 |
| G: -6727.80684 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12993.51830 HOMO: -6.05453 LUMO: -0.51157 factor:1 | 1 (-1.34577) | -1 | -1 |
| G: -6727.80684 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12992.71777 HOMO: -7.53755 LUMO: -0.38912 factor:1 | 1 (-0.54523) | 1 | 1 |
| G: -6727.80684 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12992.66895 HOMO: -7.00421 LUMO: -0.50885 factor:1 | 1 (-0.49642) | -1 | -1 |
| G: -6727.80684 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12992.93927 HOMO: -7.52123 LUMO: -0.37552 factor:1 | 1 (-0.76674) | 1 | 1 |
| G: -6727.80684 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12992.96441 HOMO: -6.70489 LUMO: -1.04764 factor:1 | 1 (-0.79188) | -1 | -1 |
| G: -6727.80684 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12993.05720 HOMO: -7.06408 LUMO: -1.16737 factor:1 | 1 (-0.88467) | 1 | 1 |
| G: -6727.80684 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12992.96289 HOMO: -6.71849 LUMO: -1.02315 factor:1 | 1 (-0.79035) | -1 | -1 |
| G: -6727.80684 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12993.13761 HOMO: -6.16610 LUMO: -0.50885 factor:1 | 1 (-0.96508) | -1 | -1 |
| G: -6727.80684 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12993.08324 HOMO: -6.48447 LUMO: 0.07619 factor:1 | 1 (-0.91071) | -1 | -1 |
| G: -6727.80684 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12993.07402 HOMO: -7.06135 LUMO: 0.09796 factor:1 | 1 (-0.90149) | 1 | 1 |
| G: -6727.80684 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12993.14670 HOMO: -6.47359 LUMO: 0.22585 factor:1 | 1 (-0.97417) | -1 | -1 |
| G: -6727.80684 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12992.95418 HOMO: -6.10896 LUMO: -0.62314 factor:1 | 1 (-0.78165) | -1 | -1 |
| G: -6727.80684 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12992.95040 HOMO: -6.88176 LUMO: -0.96600 factor:1 | 1 (-0.77786) | -1 | -1 |
| G: -6727.80684 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12993.12912 HOMO: -6.67495 LUMO: 0.21769 factor:1 | 1 (-0.95659) | -1 | -1 |
| G: -6727.80684 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12993.10234 HOMO: -6.84911 LUMO: 0.38368 factor:1 | 1 (-0.92981) | -1 | -1 |
| G: -6727.80684 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12993.22684 HOMO: -6.83550 LUMO: 1.29798 factor:1 | 1 (-1.05431) | -1 | -1 |
| G: -6727.80684 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12991.83342 HOMO: -6.67495 LUMO: 1.46941 factor:1 | -1 (0.33911) | -1 | -1 |
| G: -6727.80684 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12992.73692 HOMO: -6.81917 LUMO: 1.30887 factor:1 | 1 (-0.56439) | -1 | -1 |
| G: -6727.80684 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12993.36311 HOMO: -6.56611 LUMO: 0.66396 factor:1 | 1 (-1.19058) | -1 | -1 |
| G: -6727.80684 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12993.15456 HOMO: -6.76203 LUMO: 0.60137 factor:1 | 1 (-0.98203) | -1 | -1 |
| G: -6727.80684 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12991.96494 HOMO: -6.55794 LUMO: 0.34286 factor:1 | -1 (0.20760) | -1 | -1 |
| G: -6727.80684 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12992.24483 HOMO: -6.83550 LUMO: 0.35919 factor:1 | 1 (-0.07230) | -1 | -1 |
| G: -6727.80684 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12992.74364 HOMO: -7.17836 LUMO: 0.63130 factor:1 | 1 (-0.57111) | 1 | 1 |
| G: -6727.80684 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12993.31473 HOMO: -6.29944 LUMO: -0.69389 factor:1 | 1 (-1.14220) | -1 | -1 |
| G: -6727.80684 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12992.81997 HOMO: -7.06680 LUMO: -0.95784 factor:1 | 1 (-0.64744) | 1 | 1 |
| G: -6727.80684 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12993.18172 HOMO: -6.84638 LUMO: -0.87076 factor:1 | 1 (-1.00919) | -1 | -1 |
| G: -6727.80684 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12991.93666 HOMO: -6.96339 LUMO: -1.05308 factor:1 | -1 (0.23587) | -1 | -1 |
| G: -6727.80684 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12992.02654 HOMO: -6.75387 LUMO: -1.04220 factor:1 | -1 (0.14599) | -1 | -1 |
| G: -6727.80684 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12992.69602 HOMO: -6.71849 LUMO: -0.84355 factor:1 | 1 (-0.52349) | -1 | -1 |
| G: -6727.80684 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12992.91317 HOMO: -7.16748 LUMO: 0.51702 factor:1 | 1 (-0.74064) | 1 | 1 |
| G: -6727.80684 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12992.66057 HOMO: -6.92530 LUMO: 0.71566 factor:1 | 1 (-0.48804) | -1 | -1 |
| G: -6727.80684 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12992.14464 HOMO: -7.11034 LUMO: 0.01905 factor:1 | -1 (0.02789) | 1 | -1 |
| G: -6727.80684 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12993.40747 HOMO: -6.79468 LUMO: 0.77008 factor:1 | 1 (-1.23493) | -1 | -1 |
| G: -6727.80684 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12992.72620 HOMO: -6.52801 LUMO: 0.98233 factor:1 | 1 (-0.55367) | -1 | -1 |
| G: -6727.80684 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12993.27057 HOMO: -6.76475 LUMO: 0.53334 factor:1 | 1 (-1.09803) | -1 | -1 |
| G: -6727.80684 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12992.74313 HOMO: -5.29261 LUMO: 0.57416 factor:1 | 1 (-0.57060) | -1 | -1 |
| G: -6727.80684 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12992.51137 HOMO: -6.57971 LUMO: 0.12789 factor:1 | 1 (-0.33884) | -1 | -1 |
| G: -6727.80684 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12992.96044 HOMO: -6.99333 LUMO: 0.51430 factor:1 | 1 (-0.78791) | -1 | -1 |
| G: -6727.80684 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12992.61692 HOMO: -6.41917 LUMO: 0.19048 factor:1 | 1 (-0.44439) | -1 | -1 |
| G: -6727.80684 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12993.48921 HOMO: -6.16066 LUMO: 1.77146 factor:1 | 1 (-1.31668) | -1 | -1 |
| G: -6727.80684 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12992.50769 HOMO: -6.90353 LUMO: 1.65717 factor:1 | 1 (-0.33516) | -1 | -1 |
| G: -6727.80684 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12990.37307 HOMO: -5.94569 LUMO: 1.29526 factor:1 | -1 (1.79946) | -1 | -1 |
| G: -6727.80684 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12992.87396 HOMO: -6.60420 LUMO: 1.33880 factor:1 | 1 (-0.70143) | -1 | -1 |
| G: -6727.80684 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12992.96670 HOMO: -6.23957 LUMO: 0.09524 factor:1 | 1 (-0.79416) | -1 | -1 |
| G: -6727.80684 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12992.62146 HOMO: -6.80013 LUMO: 1.34696 factor:1 | 1 (-0.44893) | -1 | -1 |
| G: -6727.80684 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12991.69704 HOMO: -7.53483 LUMO: -1.52384 factor:1 | -1 (0.47549) | -1 | -1 |
| G: -6323.77887 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12588.02195 HOMO: -7.62463 LUMO: -1.65717 factor:1 | -1 (0.12261) | -1 | -1 |
| G: -6323.77887 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12588.08797 HOMO: -7.62463 LUMO: -1.61364 factor:1 | -1 (0.05660) | -1 | -1 |
| G: -6323.77887 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12588.15719 HOMO: -8.04096 LUMO: -1.66806 factor:1 | 1 (-0.01263) | -1 | -1 |
| G: -6323.77887 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.78918 HOMO: -7.18381 LUMO: -1.17553 factor:1 | -1 (0.35538) | 1 | 1 |
| G: -6323.77887 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.85993 HOMO: -7.69538 LUMO: -1.36601 factor:1 | -1 (0.28463) | 1 | 1 |
| G: -6323.77887 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.69441 HOMO: -7.95117 LUMO: -1.48302 factor:1 | -1 (0.45016) | -1 | -1 |
| G: -6323.77887 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12588.07695 HOMO: -6.98516 LUMO: 0.35919 factor:1 | -1 (0.06762) | -1 | -1 |
| G: -6323.77887 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12588.08105 HOMO: -7.91579 LUMO: -0.32109 factor:1 | -1 (0.06351) | 1 | 1 |
| G: -6323.77887 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.76791 HOMO: -6.75659 LUMO: -0.03537 factor:1 | -1 (0.37666) | -1 | -1 |
| G: -6323.77887 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.67101 HOMO: -7.78518 LUMO: -2.36467 factor:1 | -1 (0.47356) | -1 | -1 |
| G: -6323.77887 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.88989 HOMO: -7.96477 LUMO: -2.75651 factor:1 | -1 (0.25467) | -1 | -1 |
| G: -6323.77887 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.50722 HOMO: -7.60286 LUMO: -2.35106 factor:1 | -1 (0.63735) | -1 | -1 |
| G: -6323.77887 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.67724 HOMO: -7.38245 LUMO: -1.21635 factor:1 | -1 (0.46733) | 1 | 1 |
| G: -6323.77887 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.71941 HOMO: -7.91579 LUMO: -1.50479 factor:1 | -1 (0.42515) | -1 | -1 |
| G: -6323.77887 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.84644 HOMO: -8.07362 LUMO: -0.28028 factor:1 | -1 (0.29813) | 1 | 1 |
| G: -6323.77887 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.95455 HOMO: -7.38245 LUMO: -1.15921 factor:1 | -1 (0.19002) | 1 | 1 |
| G: -6323.77887 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.61090 HOMO: -7.18653 LUMO: -0.94968 factor:1 | -1 (0.53367) | 1 | 1 |
| G: -6323.77887 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.66499 HOMO: -6.88448 LUMO: 0.38096 factor:1 | -1 (0.47957) | -1 | -1 |
| G: -6323.77887 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.86538 HOMO: -6.97972 LUMO: 0.43266 factor:1 | -1 (0.27919) | -1 | -1 |
| G: -6323.77887 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.86747 HOMO: -6.88992 LUMO: -0.43538 factor:1 | -1 (0.27709) | -1 | -1 |
| G: -6323.77887 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.76527 HOMO: -7.97021 LUMO: -0.17143 factor:1 | -1 (0.37930) | 1 | 1 |
| G: -6323.77887 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12588.05330 HOMO: -6.92530 LUMO: 0.77280 factor:1 | -1 (0.09127) | -1 | -1 |
| G: -6323.77887 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.67560 HOMO: -7.89674 LUMO: -0.09796 factor:1 | -1 (0.46896) | 1 | 1 |
| G: -6323.77887 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.47318 HOMO: -7.02870 LUMO: 0.88709 factor:1 | -1 (0.67139) | -1 | -1 |
| G: -6323.77887 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.61928 HOMO: -6.78380 LUMO: 0.22041 factor:1 | -1 (0.52529) | -1 | -1 |
| G: -6323.77887 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.67305 HOMO: -7.24911 LUMO: -0.82178 factor:1 | -1 (0.47152) | 1 | 1 |
| G: -6323.77887 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.66535 HOMO: -6.77019 LUMO: 0.52790 factor:1 | -1 (0.47922) | -1 | -1 |
| G: -6323.77887 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.56717 HOMO: -8.56070 LUMO: -1.83405 factor:1 | -1 (0.57740) | -1 | -1 |
| G: -6323.77887 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.44978 HOMO: -7.74164 LUMO: -2.36195 factor:1 | -1 (0.69479) | -1 | -1 |
| G: -6323.77887 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.25987 HOMO: -7.39878 LUMO: -2.41637 factor:1 | -1 (0.88470) | -1 | -1 |
| G: -6323.77887 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.42795 HOMO: -7.61647 LUMO: -2.34018 factor:1 | -1 (0.71661) | -1 | -1 |
| G: -6323.77887 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12588.04734 HOMO: -6.93346 LUMO: -0.57688 factor:1 | -1 (0.09723) | -1 | -1 |
| G: -6323.77887 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.75074 HOMO: -6.85183 LUMO: -1.00410 factor:1 | -1 (0.39383) | -1 | -1 |
| G: -6323.77887 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.73574 HOMO: -7.18925 LUMO: -1.12655 factor:1 | -1 (0.40882) | 1 | 1 |
| G: -6323.77887 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.98834 HOMO: -6.85183 LUMO: -1.60275 factor:1 | -1 (0.15622) | -1 | -1 |
| G: -6323.77887 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.66102 HOMO: -7.51578 LUMO: 0.12517 factor:1 | -1 (0.48355) | 1 | 1 |
| G: -6323.77887 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.83457 HOMO: -7.36068 LUMO: 0.05714 factor:1 | -1 (0.30999) | 1 | 1 |
| G: -6323.77887 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.92976 HOMO: -7.49674 LUMO: 0.18776 factor:1 | -1 (0.21481) | 1 | 1 |
| G: -6323.77887 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.78118 HOMO: -7.09401 LUMO: -1.24900 factor:1 | -1 (0.36338) | 1 | 1 |
| G: -6323.77887 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.50357 HOMO: -7.22462 LUMO: -1.61364 factor:1 | -1 (0.64099) | -1 | -1 |
| G: -6323.77887 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.41321 HOMO: -7.74436 LUMO: -0.18776 factor:1 | -1 (0.73136) | 1 | 1 |
| G: -6323.77887 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.73063 HOMO: -7.35252 LUMO: 0.75376 factor:1 | -1 (0.41394) | 1 | 1 |
| G: -6323.77887 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.59851 HOMO: -7.75252 LUMO: 0.00816 factor:1 | -1 (0.54605) | 1 | 1 |
| G: -6323.77887 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.74622 HOMO: -7.06680 LUMO: 0.24490 factor:1 | -1 (0.39835) | 1 | 1 |
| G: -6323.77887 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.70526 HOMO: -7.49129 LUMO: 0.14150 factor:1 | -1 (0.43930) | 1 | 1 |
| G: -6323.77887 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.59541 HOMO: -6.90625 LUMO: -1.11295 factor:1 | -1 (0.54915) | -1 | -1 |
| G: -6323.77887 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.94924 HOMO: -6.78380 LUMO: -0.93063 factor:1 | -1 (0.19532) | -1 | -1 |
| G: -6323.77887 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.73642 HOMO: -7.79878 LUMO: 0.30477 factor:1 | -1 (0.40814) | 1 | 1 |
| G: -6323.77887 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.66611 HOMO: -7.87498 LUMO: 0.61770 factor:1 | -1 (0.47846) | 1 | 1 |
| G: -6323.77887 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.60837 HOMO: -7.23823 LUMO: 0.30205 factor:1 | -1 (0.53620) | 1 | 1 |
| G: -6323.77887 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.43944 HOMO: -7.67633 LUMO: 0.13061 factor:1 | -1 (0.70513) | 1 | 1 |
| G: -6323.77887 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.51274 HOMO: -7.79606 LUMO: 0.34558 factor:1 | -1 (0.63182) | 1 | 1 |
| G: -6323.77887 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.68897 HOMO: -6.66135 LUMO: -2.60141 factor:1 | -1 (0.45560) | -1 | -1 |
| G: -6323.77887 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.72317 HOMO: -7.03142 LUMO: 0.50885 factor:1 | -1 (0.42140) | -1 | -1 |
| G: -6323.77887 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.83591 HOMO: -7.05591 LUMO: -0.06531 factor:1 | -1 (0.30866) | -1 | -1 |
| G: -6323.77887 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.56306 HOMO: -7.45592 LUMO: -1.39594 factor:1 | -1 (0.58151) | 1 | 1 |
| G: -6323.77887 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.43650 HOMO: -7.22462 LUMO: -1.10478 factor:1 | -1 (0.70807) | 1 | 1 |
| G: -6323.77887 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.40510 HOMO: -8.14709 LUMO: -0.55783 factor:1 | -1 (0.73947) | 1 | 1 |
| G: -6323.77887 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.20942 HOMO: -7.22190 LUMO: -1.14560 factor:1 | -1 (0.93515) | 1 | 1 |
| G: -6323.77887 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.86867 HOMO: -7.28721 LUMO: -1.14016 factor:1 | -1 (0.27590) | 1 | 1 |
| G: -6323.77887 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.75710 HOMO: -6.97156 LUMO: 0.51702 factor:1 | -1 (0.38746) | -1 | -1 |
| G: -6323.77887 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.63536 HOMO: -7.37156 LUMO: 0.29388 factor:1 | -1 (0.50921) | 1 | -1 |
| G: -6323.77887 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.64581 HOMO: -7.66273 LUMO: -1.59731 factor:1 | -1 (0.49876) | -1 | -1 |
| G: -6323.77887 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.80742 HOMO: -7.50490 LUMO: -1.49935 factor:1 | -1 (0.33715) | -1 | -1 |
| G: -6323.77887 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.69180 HOMO: -7.61102 LUMO: -1.45581 factor:1 | -1 (0.45277) | 1 | 1 |
| G: -6323.77887 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.89811 HOMO: -7.58653 LUMO: -1.61091 factor:1 | -1 (0.24645) | -1 | -1 |
| G: -6323.77887 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.84276 HOMO: -7.36068 LUMO: -1.14560 factor:1 | -1 (0.30180) | 1 | 1 |
| G: -6323.77887 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.61158 HOMO: -6.96339 LUMO: 0.26939 factor:1 | -1 (0.53299) | -1 | -1 |
| G: -6323.77887 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.52845 HOMO: -6.53617 LUMO: 0.22313 factor:1 | -1 (0.61612) | -1 | -1 |
| G: -6323.77887 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.53468 HOMO: -7.33619 LUMO: -1.02587 factor:1 | -1 (0.60989) | 1 | 1 |
| G: -6323.77887 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.42469 HOMO: -6.87904 LUMO: 0.33742 factor:1 | -1 (0.71988) | -1 | -1 |
| G: -6323.77887 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.94908 HOMO: -6.88448 LUMO: 0.58777 factor:1 | -1 (0.19549) | -1 | -1 |
| G: -6323.77887 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.71463 HOMO: -6.55522 LUMO: -1.51295 factor:1 | -1 (0.42994) | -1 | -1 |
| G: -6323.77887 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.59819 HOMO: -7.43415 LUMO: 0.10612 factor:1 | -1 (0.54638) | 1 | 1 |
| G: -6323.77887 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.76663 HOMO: -7.54300 LUMO: -0.02449 factor:1 | -1 (0.37794) | 1 | 1 |
| G: -6323.77887 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.47653 HOMO: -7.42054 LUMO: 0.28028 factor:1 | -1 (0.66804) | 1 | 1 |
| G: -6323.77887 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.49057 HOMO: -6.98244 LUMO: -0.95784 factor:1 | -1 (0.65400) | -1 | -1 |
| G: -6323.77887 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.34504 HOMO: -6.96884 LUMO: -1.12383 factor:1 | -1 (0.79952) | -1 | -1 |
| G: -6323.77887 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.61500 HOMO: -6.80829 LUMO: -0.98233 factor:1 | -1 (0.52956) | -1 | -1 |
| G: -6323.77887 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.33919 HOMO: -7.60830 LUMO: 0.58504 factor:1 | -1 (0.80538) | 1 | 1 |
| G: -6323.77887 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.33650 HOMO: -7.52123 LUMO: 0.08163 factor:1 | -1 (0.80807) | 1 | 1 |
| G: -6323.77887 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.19353 HOMO: -7.59742 LUMO: 0.00272 factor:1 | -1 (0.95104) | 1 | 1 |
| G: -6323.77887 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.33541 HOMO: -6.99333 LUMO: -1.33880 factor:1 | -1 (0.80916) | -1 | -1 |
| G: -6323.77887 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.20477 HOMO: -6.63958 LUMO: -1.39322 factor:1 | -1 (0.93980) | -1 | -1 |
| G: -6323.77887 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12586.96528 HOMO: -7.86137 LUMO: 0.01633 factor:1 | -1 (1.17929) | 1 | 1 |
| G: -6323.77887 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.44295 HOMO: -7.29537 LUMO: 0.14694 factor:1 | -1 (0.70162) | 1 | 1 |
| G: -6323.77887 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.64031 HOMO: -6.95523 LUMO: 0.48708 factor:1 | -1 (0.50425) | -1 | -1 |
| G: -6323.77887 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.83196 HOMO: -7.10217 LUMO: -1.10478 factor:1 | -1 (0.31260) | 1 | 1 |
| G: -6323.77887 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.81838 HOMO: -6.88176 LUMO: -0.96328 factor:1 | -1 (0.32618) | -1 | -1 |
| G: -6323.77887 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.61079 HOMO: -7.89130 LUMO: -0.13334 factor:1 | -1 (0.53378) | 1 | 1 |
| G: -6323.77887 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.80676 HOMO: -7.75252 LUMO: 0.25579 factor:1 | -1 (0.33780) | 1 | 1 |
| G: -6323.77887 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.81397 HOMO: -6.87632 LUMO: -0.93063 factor:1 | -1 (0.33059) | -1 | -1 |
| G: -6323.77887 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.91980 HOMO: -6.78108 LUMO: -0.86804 factor:1 | -1 (0.22477) | -1 | -1 |
| G: -6323.77887 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.69683 HOMO: -5.98106 LUMO: 0.10340 factor:1 | -1 (0.44774) | -1 | -1 |
| G: -6323.77887 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.61838 HOMO: -6.40284 LUMO: -0.87349 factor:1 | -1 (0.52619) | -1 | -1 |
| G: -6323.77887 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.60265 HOMO: -6.77019 LUMO: -1.20819 factor:1 | -1 (0.54191) | -1 | -1 |
| G: -6323.77887 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.46610 HOMO: -6.90081 LUMO: -1.00682 factor:1 | -1 (0.67846) | -1 | -1 |
| G: -6323.77887 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.39862 HOMO: -6.59060 LUMO: -0.26667 factor:1 | -1 (0.74595) | -1 | -1 |
| G: -6323.77887 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.45351 HOMO: -6.50896 LUMO: -0.48708 factor:1 | -1 (0.69106) | -1 | -1 |
| G: -6323.77887 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.47688 HOMO: -6.20420 LUMO: -0.73471 factor:1 | -1 (0.66769) | -1 | -1 |
| G: -6323.77887 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.38599 HOMO: -6.17154 LUMO: -0.68573 factor:1 | -1 (0.75857) | -1 | -1 |
| G: -6323.77887 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.67033 HOMO: -6.21236 LUMO: 0.09796 factor:1 | -1 (0.47424) | -1 | -1 |
| G: -6323.77887 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.66442 HOMO: -6.38379 LUMO: 0.58232 factor:1 | -1 (0.48014) | -1 | -1 |
| G: -6323.77887 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.67767 HOMO: -7.42871 LUMO: 0.40273 factor:1 | -1 (0.46689) | 1 | 1 |
| G: -6323.77887 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.59743 HOMO: -6.54978 LUMO: 0.26395 factor:1 | -1 (0.54714) | -1 | -1 |
| G: -6323.77887 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.35639 HOMO: -7.14027 LUMO: 0.14150 factor:1 | -1 (0.78818) | 1 | 1 |
| G: -6323.77887 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.45541 HOMO: -7.25456 LUMO: -0.15783 factor:1 | -1 (0.68916) | 1 | 1 |
| G: -6323.77887 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.39625 HOMO: -6.90897 LUMO: 0.63403 factor:1 | -1 (0.74831) | -1 | -1 |
| G: -6323.77887 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.25522 HOMO: -6.49264 LUMO: 0.71022 factor:1 | -1 (0.88935) | -1 | -1 |
| G: -6323.77887 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.51952 HOMO: -6.56067 LUMO: -1.03947 factor:1 | -1 (0.62505) | -1 | -1 |
| G: -6323.77887 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.83389 HOMO: -6.79196 LUMO: -1.12655 factor:1 | -1 (0.31067) | -1 | -1 |
| G: -6323.77887 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.53892 HOMO: -6.95251 LUMO: -1.09118 factor:1 | -1 (0.60564) | -1 | -1 |
| G: -6323.77887 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.59070 HOMO: -7.47225 LUMO: -0.22041 factor:1 | -1 (0.55386) | 1 | 1 |
| G: -6323.77887 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.66608 HOMO: -7.13483 LUMO: -0.98505 factor:1 | -1 (0.47849) | 1 | 1 |
| G: -6323.77887 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.74687 HOMO: -6.99061 LUMO: -1.05852 factor:1 | -1 (0.39769) | -1 | -1 |
| G: -6323.77887 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.70246 HOMO: -6.52257 LUMO: -1.11022 factor:1 | -1 (0.44210) | -1 | -1 |
| G: -6323.77887 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.38719 HOMO: -6.75114 LUMO: -1.09934 factor:1 | -1 (0.75737) | -1 | -1 |
| G: -6323.77887 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.54673 HOMO: -6.82189 LUMO: -0.89253 factor:1 | -1 (0.59783) | -1 | -1 |
| G: -6323.77887 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.38009 HOMO: -6.83278 LUMO: -0.97961 factor:1 | -1 (0.76448) | -1 | -1 |
| G: -6323.77887 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.74995 HOMO: -6.65318 LUMO: -0.84355 factor:1 | -1 (0.39462) | -1 | -1 |
| G: -6323.77887 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.69033 HOMO: -6.75931 LUMO: -0.88437 factor:1 | -1 (0.45424) | -1 | -1 |
| G: -6323.77887 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.63841 HOMO: -6.19059 LUMO: -0.45715 factor:1 | -1 (0.50616) | -1 | -1 |
| G: -6323.77887 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.36512 HOMO: -7.09673 LUMO: -2.01908 factor:1 | -1 (0.77944) | -1 | -1 |
| G: -6323.77887 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.43827 HOMO: -7.88042 LUMO: 0.38640 factor:1 | -1 (0.70630) | 1 | 1 |
| G: -6323.77887 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.30986 HOMO: -7.83144 LUMO: 0.14422 factor:1 | -1 (0.83471) | 1 | 1 |
| G: -6323.77887 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.19628 HOMO: -7.46408 LUMO: 0.44627 factor:1 | -1 (0.94829) | 1 | 1 |
| G: -6323.77887 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12586.98457 HOMO: -7.12394 LUMO: -2.04902 factor:1 | -1 (1.15999) | -1 | -1 |
| G: -6323.77887 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.52787 HOMO: -6.78380 LUMO: -1.11295 factor:1 | -1 (0.61669) | -1 | -1 |
| G: -6323.77887 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.40319 HOMO: -7.12938 LUMO: -0.23674 factor:1 | -1 (0.74137) | 1 | 1 |
| G: -6324.15077 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12588.02195 HOMO: -6.14705 LUMO: -0.20409 factor:1 | -1 (0.49451) | -1 | -1 |
| G: -6324.15077 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12588.08797 HOMO: -6.50080 LUMO: -0.28300 factor:1 | -1 (0.42850) | -1 | -1 |
| G: -6324.15077 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12588.15719 HOMO: -6.50352 LUMO: -0.62042 factor:1 | -1 (0.35927) | -1 | -1 |
| G: -6324.15077 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.78918 HOMO: -6.46543 LUMO: -0.53879 factor:1 | -1 (0.72728) | -1 | -1 |
| G: -6324.15077 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.85993 HOMO: -7.32803 LUMO: -0.52790 factor:1 | -1 (0.65653) | 1 | 1 |
| G: -6324.15077 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.69441 HOMO: -5.94025 LUMO: -0.17687 factor:1 | -1 (0.82206) | -1 | -1 |
| G: -6324.15077 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12588.07695 HOMO: -5.62187 LUMO: 0.05714 factor:1 | -1 (0.43952) | -1 | -1 |
| G: -6324.15077 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12588.08105 HOMO: -7.03414 LUMO: -1.04492 factor:1 | -1 (0.43541) | -1 | -1 |
| G: -6324.15077 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.76791 HOMO: -6.75387 LUMO: -2.02181 factor:1 | -1 (0.74856) | -1 | -1 |
| G: -6324.15077 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.67101 HOMO: -6.55250 LUMO: -0.75648 factor:1 | -1 (0.84546) | -1 | -1 |
| G: -6324.15077 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.88989 HOMO: -6.81101 LUMO: -1.02043 factor:1 | -1 (0.62657) | -1 | -1 |
| G: -6324.15077 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.50722 HOMO: -6.69672 LUMO: -2.81910 factor:1 | -1 (1.00924) | -1 | -1 |
| G: -6324.15077 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.67724 HOMO: -6.69128 LUMO: -2.58236 factor:1 | -1 (0.83923) | -1 | -1 |
| G: -6324.15077 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.71941 HOMO: -6.73482 LUMO: -2.06807 factor:1 | -1 (0.79705) | -1 | -1 |
| G: -6324.15077 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.84644 HOMO: -7.66545 LUMO: 0.17143 factor:1 | -1 (0.67003) | 1 | 1 |
| G: -6324.15077 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.95455 HOMO: -6.87904 LUMO: -1.25172 factor:1 | -1 (0.56192) | -1 | -1 |
| G: -6324.15077 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.61090 HOMO: -6.84366 LUMO: -0.19320 factor:1 | -1 (0.90557) | -1 | -1 |
| G: -6324.15077 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.66499 HOMO: -6.97972 LUMO: -0.97961 factor:1 | -1 (0.85147) | -1 | -1 |
| G: -6324.15077 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.86538 HOMO: -6.72121 LUMO: -0.70477 factor:1 | -1 (0.65109) | -1 | -1 |
| G: -6324.15077 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.86747 HOMO: -7.18925 LUMO: 0.40001 factor:1 | -1 (0.64899) | 1 | 1 |
| G: -6324.15077 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.76527 HOMO: -6.72121 LUMO: 0.19592 factor:1 | -1 (0.75120) | -1 | -1 |
| G: -6324.15077 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12588.05330 HOMO: -6.85999 LUMO: -0.39457 factor:1 | -1 (0.46317) | -1 | -1 |
| G: -6324.15077 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.67560 HOMO: -6.90625 LUMO: 0.05987 factor:1 | -1 (0.84086) | -1 | -1 |
| G: -6324.15077 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.47318 HOMO: -7.00421 LUMO: 0.37552 factor:1 | -1 (1.04328) | -1 | -1 |
| G: -6324.15077 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.61928 HOMO: -6.56883 LUMO: -0.97689 factor:1 | -1 (0.89719) | -1 | -1 |
| G: -6324.15077 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.67305 HOMO: -6.66679 LUMO: 0.56055 factor:1 | -1 (0.84342) | -1 | -1 |
| G: -6324.15077 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.66535 HOMO: -6.75931 LUMO: 0.32926 factor:1 | -1 (0.85112) | -1 | -1 |
| G: -6324.15077 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.56717 HOMO: -6.53617 LUMO: -1.06397 factor:1 | -1 (0.94930) | -1 | -1 |
| G: -6324.15077 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.44978 HOMO: -6.78108 LUMO: 0.42722 factor:1 | -1 (1.06669) | -1 | -1 |
| G: -6324.15077 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.25987 HOMO: -7.05319 LUMO: 0.61498 factor:1 | -1 (1.25659) | -1 | -1 |
| G: -6324.15077 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.42795 HOMO: -6.78380 LUMO: 1.49391 factor:1 | -1 (1.08851) | -1 | -1 |
| G: -6324.15077 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12588.04734 HOMO: -7.21102 LUMO: 0.27211 factor:1 | -1 (0.46912) | 1 | 1 |
| G: -6324.15077 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.75074 HOMO: -6.67223 LUMO: 0.81362 factor:1 | -1 (0.76573) | -1 | -1 |
| G: -6324.15077 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.73574 HOMO: -6.69944 LUMO: 1.40683 factor:1 | -1 (0.78072) | -1 | -1 |
| G: -6324.15077 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.98834 HOMO: -7.02598 LUMO: 1.46941 factor:1 | -1 (0.52812) | -1 | -1 |
| G: -6324.15077 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.66102 HOMO: -5.85045 LUMO: -0.76736 factor:1 | -1 (0.85544) | -1 | -1 |
| G: -6324.15077 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.83457 HOMO: -6.53890 LUMO: -0.50885 factor:1 | -1 (0.68189) | -1 | -1 |
| G: -6324.15077 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.92976 HOMO: -6.42733 LUMO: -0.63947 factor:1 | -1 (0.58670) | -1 | -1 |
| G: -6324.15077 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.78118 HOMO: -6.82189 LUMO: -0.85444 factor:1 | -1 (0.73528) | -1 | -1 |
| G: -6324.15077 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.50357 HOMO: -6.97428 LUMO: -1.22179 factor:1 | -1 (1.01289) | -1 | -1 |
| G: -6324.15077 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.41321 HOMO: -6.93346 LUMO: -1.09934 factor:1 | -1 (1.10326) | -1 | -1 |
| G: -6324.15077 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.73063 HOMO: -7.17292 LUMO: -1.11839 factor:1 | -1 (0.78584) | 1 | 1 |
| G: -6324.15077 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.59851 HOMO: -7.00965 LUMO: -1.23268 factor:1 | -1 (0.91795) | -1 | -1 |
| G: -6324.15077 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.74622 HOMO: -6.73210 LUMO: -1.12383 factor:1 | -1 (0.77025) | -1 | -1 |
| G: -6324.15077 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.70526 HOMO: -7.61375 LUMO: -0.11973 factor:1 | -1 (0.81120) | 1 | 1 |
| G: -6324.15077 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.59541 HOMO: -7.42327 LUMO: 0.41906 factor:1 | -1 (0.92105) | 1 | 1 |
| G: -6324.15077 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.94924 HOMO: -6.94162 LUMO: -1.01771 factor:1 | -1 (0.56722) | -1 | -1 |
| G: -6324.15077 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.73642 HOMO: -6.82189 LUMO: -0.92791 factor:1 | -1 (0.78004) | -1 | -1 |
| G: -6324.15077 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.66611 HOMO: -6.92258 LUMO: -1.73881 factor:1 | -1 (0.85036) | -1 | -1 |
| G: -6324.15077 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.60837 HOMO: -6.50896 LUMO: -1.60819 factor:1 | -1 (0.90810) | -1 | -1 |
| G: -6324.15077 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.43944 HOMO: -6.38379 LUMO: -2.18780 factor:1 | -1 (1.07703) | -1 | -1 |
| G: -6324.15077 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.51274 HOMO: -6.48992 LUMO: -0.97417 factor:1 | -1 (1.00372) | -1 | -1 |
| G: -6324.15077 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.68897 HOMO: -6.01644 LUMO: -0.04354 factor:1 | -1 (0.82750) | -1 | -1 |
| G: -6324.15077 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.72317 HOMO: -6.70761 LUMO: -0.14422 factor:1 | -1 (0.79329) | -1 | -1 |
| G: -6324.15077 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.83591 HOMO: -6.70216 LUMO: 0.14422 factor:1 | -1 (0.68056) | -1 | -1 |
| G: -6324.15077 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.56306 HOMO: -7.07224 LUMO: -0.10885 factor:1 | -1 (0.95341) | 1 | 1 |
| G: -6324.15077 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.43650 HOMO: -7.52667 LUMO: -0.74287 factor:1 | -1 (1.07997) | 1 | 1 |
| G: -6324.15077 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.40510 HOMO: -6.48447 LUMO: -0.96056 factor:1 | -1 (1.11137) | -1 | -1 |
| G: -6324.15077 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.20942 HOMO: -6.22597 LUMO: -0.41361 factor:1 | -1 (1.30704) | -1 | -1 |
| G: -6324.15077 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.86867 HOMO: -6.12256 LUMO: -1.05852 factor:1 | -1 (0.64779) | -1 | -1 |
| G: -6324.15077 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.75710 HOMO: -6.97428 LUMO: -0.60681 factor:1 | -1 (0.75936) | -1 | -1 |
| G: -6324.15077 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.63536 HOMO: -6.78380 LUMO: -0.88981 factor:1 | -1 (0.88110) | -1 | -1 |
| G: -6324.15077 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.64581 HOMO: -6.85999 LUMO: 0.07891 factor:1 | -1 (0.87066) | -1 | -1 |
| G: -6324.15077 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.80742 HOMO: -7.08312 LUMO: -0.60137 factor:1 | -1 (0.70905) | 1 | 1 |
| G: -6324.15077 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.69180 HOMO: -6.57699 LUMO: -0.68028 factor:1 | -1 (0.82467) | -1 | -1 |
| G: -6324.15077 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.89811 HOMO: -6.09807 LUMO: -0.31837 factor:1 | -1 (0.61835) | -1 | -1 |
| G: -6324.15077 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.84276 HOMO: -6.10624 LUMO: 0.14966 factor:1 | -1 (0.67370) | -1 | -1 |
| G: -6324.15077 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.61158 HOMO: -6.77019 LUMO: -0.95784 factor:1 | -1 (0.90489) | -1 | -1 |
| G: -6324.15077 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.52845 HOMO: -5.93208 LUMO: -0.44627 factor:1 | -1 (0.98802) | -1 | -1 |
| G: -6324.15077 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.53468 HOMO: -6.12256 LUMO: -0.27756 factor:1 | -1 (0.98179) | -1 | -1 |
| G: -6324.15077 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.42469 HOMO: -5.98106 LUMO: -0.37824 factor:1 | -1 (1.09178) | -1 | -1 |
| G: -6324.15077 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.94908 HOMO: -7.06408 LUMO: -1.12927 factor:1 | -1 (0.56738) | 1 | 1 |
| G: -6324.15077 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.71463 HOMO: -6.70761 LUMO: -0.98505 factor:1 | -1 (0.80184) | -1 | -1 |
| G: -6324.15077 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.59819 HOMO: -7.00965 LUMO: -0.42722 factor:1 | -1 (0.91828) | -1 | -1 |
| G: -6324.15077 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.76663 HOMO: -5.96201 LUMO: -0.59049 factor:1 | -1 (0.74984) | -1 | -1 |
| G: -6324.15077 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.47653 HOMO: -6.34570 LUMO: -1.68438 factor:1 | -1 (1.03994) | -1 | -1 |
| G: -6324.15077 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.49057 HOMO: -6.97156 LUMO: -1.85854 factor:1 | -1 (1.02590) | -1 | -1 |
| G: -6324.15077 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.34504 HOMO: -5.91848 LUMO: -2.51433 factor:1 | -1 (1.17142) | -1 | -1 |
| G: -6324.15077 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.61500 HOMO: -6.39195 LUMO: -1.66262 factor:1 | -1 (0.90146) | -1 | -1 |
| G: -6324.15077 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.33919 HOMO: -6.50352 LUMO: 0.19592 factor:1 | -1 (1.17727) | -1 | -1 |
| G: -6324.15077 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.33650 HOMO: -6.45998 LUMO: 0.34831 factor:1 | -1 (1.17997) | -1 | -1 |
| G: -6324.15077 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.19353 HOMO: -7.05319 LUMO: 0.23402 factor:1 | -1 (1.32294) | -1 | -1 |
| G: -6324.15077 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.33541 HOMO: -6.61237 LUMO: 0.18232 factor:1 | -1 (1.18106) | -1 | -1 |
| G: -6324.15077 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.20477 HOMO: -6.57427 LUMO: 0.40545 factor:1 | -1 (1.31170) | -1 | -1 |
| G: -6324.15077 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12586.96528 HOMO: -7.26544 LUMO: 0.41089 factor:1 | -1 (1.55119) | 1 | 1 |
| G: -6324.15077 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.44295 HOMO: -6.26406 LUMO: -0.85444 factor:1 | -1 (1.07352) | -1 | -1 |
| G: -6324.15077 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.64031 HOMO: -6.25318 LUMO: -0.79457 factor:1 | -1 (0.87615) | -1 | -1 |
| G: -6324.15077 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.83196 HOMO: -6.68040 LUMO: 0.41089 factor:1 | -1 (0.68450) | -1 | -1 |
| G: -6324.15077 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.81838 HOMO: -6.37835 LUMO: 0.37280 factor:1 | -1 (0.69808) | -1 | -1 |
| G: -6324.15077 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.61079 HOMO: -6.56067 LUMO: 0.62858 factor:1 | -1 (0.90568) | -1 | -1 |
| G: -6324.15077 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.80676 HOMO: -6.74026 LUMO: -0.04082 factor:1 | -1 (0.70970) | -1 | -1 |
| G: -6324.15077 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.81397 HOMO: -6.53617 LUMO: 0.35103 factor:1 | -1 (0.70249) | -1 | -1 |
| G: -6324.15077 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.91980 HOMO: -6.51985 LUMO: 0.25851 factor:1 | -1 (0.59666) | -1 | -1 |
| G: -6324.15077 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.69683 HOMO: -6.58788 LUMO: -1.98371 factor:1 | -1 (0.81963) | -1 | -1 |
| G: -6324.15077 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.61838 HOMO: -6.51441 LUMO: 0.29116 factor:1 | -1 (0.89808) | -1 | -1 |
| G: -6324.15077 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.60265 HOMO: -6.81101 LUMO: 0.35647 factor:1 | -1 (0.91381) | -1 | -1 |
| G: -6324.15077 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.46610 HOMO: -6.42733 LUMO: 0.10340 factor:1 | -1 (1.05036) | -1 | -1 |
| G: -6324.15077 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.39862 HOMO: -6.70761 LUMO: 0.28028 factor:1 | -1 (1.11784) | -1 | -1 |
| G: -6324.15077 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.45351 HOMO: -6.67495 LUMO: 0.01633 factor:1 | -1 (1.06296) | -1 | -1 |
| G: -6324.15077 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.47688 HOMO: -6.75387 LUMO: 0.15510 factor:1 | -1 (1.03958) | -1 | -1 |
| G: -6324.15077 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.38599 HOMO: -6.56067 LUMO: 0.35919 factor:1 | -1 (1.13047) | -1 | -1 |
| G: -6324.15077 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.67033 HOMO: -7.16748 LUMO: 0.21497 factor:1 | -1 (0.84614) | 1 | 1 |
| G: -6324.15077 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.66442 HOMO: -6.71849 LUMO: 0.26667 factor:1 | -1 (0.85204) | -1 | -1 |
| G: -6324.15077 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.67767 HOMO: -6.69128 LUMO: 0.55783 factor:1 | -1 (0.83879) | -1 | -1 |
| G: -6324.15077 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.59743 HOMO: -6.71305 LUMO: 0.45987 factor:1 | -1 (0.91904) | -1 | -1 |
| G: -6324.15077 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.35639 HOMO: -5.90487 LUMO: -0.70750 factor:1 | -1 (1.16008) | -1 | -1 |
| G: -6324.15077 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.45541 HOMO: -6.84638 LUMO: -0.72110 factor:1 | -1 (1.06105) | -1 | -1 |
| G: -6324.15077 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.39625 HOMO: -6.66135 LUMO: -1.13471 factor:1 | -1 (1.12021) | -1 | -1 |
| G: -6324.15077 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.25522 HOMO: -6.74026 LUMO: -0.64763 factor:1 | -1 (1.26125) | -1 | -1 |
| G: -6324.15077 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.51952 HOMO: -6.69672 LUMO: -1.05036 factor:1 | -1 (0.99694) | -1 | -1 |
| G: -6324.15077 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.83389 HOMO: -6.78924 LUMO: -1.03675 factor:1 | -1 (0.68257) | -1 | -1 |
| G: -6324.15077 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.53892 HOMO: -6.81373 LUMO: -0.85988 factor:1 | -1 (0.97754) | -1 | -1 |
| G: -6324.15077 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.59070 HOMO: -7.26544 LUMO: 0.91158 factor:1 | -1 (0.92576) | 1 | 1 |
| G: -6324.15077 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.66608 HOMO: -6.64230 LUMO: -1.92929 factor:1 | -1 (0.85038) | -1 | -1 |
| G: -6324.15077 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.74687 HOMO: -7.20830 LUMO: 0.11429 factor:1 | -1 (0.76959) | 1 | 1 |
| G: -6324.15077 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.70246 HOMO: -7.17020 LUMO: 0.04898 factor:1 | -1 (0.81400) | 1 | 1 |
| G: -6324.15077 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.38719 HOMO: -7.16476 LUMO: 0.04898 factor:1 | -1 (1.12927) | 1 | 1 |
| G: -6324.15077 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.54673 HOMO: -6.59332 LUMO: -0.49253 factor:1 | -1 (0.96973) | -1 | -1 |
| G: -6324.15077 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.38009 HOMO: -7.46953 LUMO: 0.84083 factor:1 | -1 (1.13637) | 1 | 1 |
| G: -6324.15077 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.74995 HOMO: -7.39878 LUMO: 0.88709 factor:1 | -1 (0.76652) | 1 | 1 |
| G: -6324.15077 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.69033 HOMO: -6.84094 LUMO: -0.61498 factor:1 | -1 (0.82614) | -1 | -1 |
| G: -6324.15077 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.63841 HOMO: -6.03549 LUMO: -0.27211 factor:1 | -1 (0.87806) | -1 | -1 |
| G: -6324.15077 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.36512 HOMO: -7.31170 LUMO: -0.64763 factor:1 | -1 (1.15134) | 1 | 1 |
| G: -6324.15077 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.43827 HOMO: -6.88992 LUMO: -0.84627 factor:1 | -1 (1.07820) | -1 | -1 |
| G: -6324.15077 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.30986 HOMO: -7.12666 LUMO: -0.09252 factor:1 | -1 (1.20661) | 1 | 1 |
| G: -6324.15077 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.19628 HOMO: -6.70489 LUMO: -0.63675 factor:1 | -1 (1.32019) | -1 | -1 |
| G: -6324.15077 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12586.98457 HOMO: -6.98788 LUMO: 0.86804 factor:1 | -1 (1.53189) | -1 | -1 |
| G: -6324.15077 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.52787 HOMO: -6.80285 LUMO: -0.60954 factor:1 | -1 (0.98859) | -1 | -1 |
| G: -6324.15077 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.40319 HOMO: -7.02054 LUMO: -0.74287 factor:1 | -1 (1.11327) | -1 | -1 |
| G: -6322.94898 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12588.02195 HOMO: -7.03686 LUMO: -0.81090 factor:1 | 1 (-0.70728) | -1 | -1 |
| G: -6322.94898 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12588.08797 HOMO: -6.70489 LUMO: -1.00954 factor:1 | 1 (-0.77329) | -1 | -1 |
| G: -6322.94898 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12588.15719 HOMO: -7.69810 LUMO: 0.00544 factor:1 | 1 (-0.84252) | 1 | 1 |
| G: -6322.94898 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.78918 HOMO: -6.83550 LUMO: -0.11157 factor:1 | 1 (-0.47451) | -1 | -1 |
| G: -6322.94898 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.85993 HOMO: -6.76203 LUMO: -2.13609 factor:1 | 1 (-0.54526) | -1 | -1 |
| G: -6322.94898 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.69441 HOMO: -6.72121 LUMO: -2.62862 factor:1 | 1 (-0.37973) | -1 | -1 |
| G: -6322.94898 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12588.07695 HOMO: -6.48719 LUMO: -2.73474 factor:1 | 1 (-0.76227) | -1 | -1 |
| G: -6322.94898 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12588.08105 HOMO: -6.83006 LUMO: -0.00544 factor:1 | 1 (-0.76638) | -1 | -1 |
| G: -6322.94898 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.76791 HOMO: -6.84094 LUMO: -1.11022 factor:1 | 1 (-0.45323) | -1 | -1 |
| G: -6322.94898 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.67101 HOMO: -6.66951 LUMO: -1.23812 factor:1 | 1 (-0.35633) | -1 | -1 |
| G: -6322.94898 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.88989 HOMO: -6.78380 LUMO: -1.27894 factor:1 | 1 (-0.57522) | -1 | -1 |
| G: -6322.94898 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.50722 HOMO: -6.50352 LUMO: -0.56055 factor:1 | 1 (-0.19255) | -1 | -1 |
| G: -6322.94898 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.67724 HOMO: -7.77974 LUMO: -0.26395 factor:1 | 1 (-0.36256) | 1 | 1 |
| G: -6322.94898 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.71941 HOMO: -7.01510 LUMO: -1.64085 factor:1 | 1 (-0.40474) | -1 | -1 |
| G: -6322.94898 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.84644 HOMO: -6.59876 LUMO: -0.91158 factor:1 | 1 (-0.53176) | -1 | -1 |
| G: -6322.94898 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.95455 HOMO: -4.67219 LUMO: -0.67756 factor:1 | 1 (-0.63988) | -1 | -1 |
| G: -6322.94898 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.61090 HOMO: -6.70489 LUMO: -0.65579 factor:1 | 1 (-0.29622) | -1 | -1 |
| G: -6322.94898 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.66499 HOMO: -6.62325 LUMO: -0.60409 factor:1 | 1 (-0.35032) | -1 | -1 |
| G: -6322.94898 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.86538 HOMO: -6.20147 LUMO: 0.15238 factor:1 | 1 (-0.55070) | -1 | -1 |
| G: -6322.94898 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.86747 HOMO: -6.43549 LUMO: -0.07075 factor:1 | 1 (-0.55280) | -1 | -1 |
| G: -6322.94898 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.76527 HOMO: -7.02054 LUMO: 0.13061 factor:1 | 1 (-0.45059) | -1 | -1 |
| G: -6322.94898 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12588.05330 HOMO: -7.04503 LUMO: 0.30749 factor:1 | 1 (-0.73863) | -1 | -1 |
| G: -6322.94898 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.67560 HOMO: -6.74842 LUMO: -0.99594 factor:1 | 1 (-0.36093) | -1 | -1 |
| G: -6322.94898 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.47318 HOMO: -6.35658 LUMO: 0.41633 factor:1 | 1 (-0.15851) | -1 | -1 |
| G: -6322.94898 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.61928 HOMO: -6.79740 LUMO: 0.56872 factor:1 | 1 (-0.30460) | -1 | -1 |
| G: -6322.94898 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.67305 HOMO: -6.51713 LUMO: -0.05987 factor:1 | 1 (-0.35837) | -1 | -1 |
| G: -6322.94898 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.66535 HOMO: -6.68040 LUMO: 0.34558 factor:1 | 1 (-0.35067) | -1 | -1 |
| G: -6322.94898 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.56717 HOMO: -6.39740 LUMO: 0.50069 factor:1 | 1 (-0.25249) | -1 | -1 |
| G: -6322.94898 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.44978 HOMO: -6.91713 LUMO: -0.97145 factor:1 | 1 (-0.13510) | -1 | -1 |
| G: -6322.94898 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.25987 HOMO: -7.10761 LUMO: -0.27483 factor:1 | -1 (0.05480) | 1 | -1 |
| G: -6322.94898 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.42795 HOMO: -6.98788 LUMO: 0.40273 factor:1 | 1 (-0.11328) | -1 | -1 |
| G: -6322.94898 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12588.04734 HOMO: -6.87087 LUMO: 0.28572 factor:1 | 1 (-0.73267) | -1 | -1 |
| G: -6322.94898 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.75074 HOMO: -7.36612 LUMO: -0.12245 factor:1 | 1 (-0.43606) | 1 | 1 |
| G: -6322.94898 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.73574 HOMO: -6.72938 LUMO: 0.33742 factor:1 | 1 (-0.42107) | -1 | -1 |
| G: -6322.94898 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.98834 HOMO: -7.32531 LUMO: 0.07619 factor:1 | 1 (-0.67367) | 1 | 1 |
| G: -6322.94898 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.66102 HOMO: -6.87087 LUMO: -0.08436 factor:1 | 1 (-0.34635) | -1 | -1 |
| G: -6322.94898 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.83457 HOMO: -6.67495 LUMO: 0.85988 factor:1 | 1 (-0.51990) | -1 | -1 |
| G: -6322.94898 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.92976 HOMO: -6.96339 LUMO: 0.65307 factor:1 | 1 (-0.61509) | -1 | -1 |
| G: -6322.94898 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.78118 HOMO: -6.58516 LUMO: -0.78641 factor:1 | 1 (-0.46651) | -1 | -1 |
| G: -6322.94898 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.50357 HOMO: -6.56883 LUMO: 0.44355 factor:1 | 1 (-0.18890) | -1 | -1 |
| G: -6322.94898 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.41321 HOMO: -6.68312 LUMO: 0.43538 factor:1 | 1 (-0.09853) | -1 | -1 |
| G: -6322.94898 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.73063 HOMO: -6.81917 LUMO: 0.20681 factor:1 | 1 (-0.41595) | -1 | -1 |
| G: -6322.94898 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.59851 HOMO: -6.91169 LUMO: 0.08163 factor:1 | 1 (-0.28384) | -1 | -1 |
| G: -6322.94898 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.74622 HOMO: -4.88444 LUMO: -0.49253 factor:1 | 1 (-0.43155) | -1 | -1 |
| G: -6322.94898 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.70526 HOMO: -6.42189 LUMO: 0.64763 factor:1 | 1 (-0.39059) | -1 | -1 |
| G: -6322.94898 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.59541 HOMO: -6.24501 LUMO: 0.55783 factor:1 | 1 (-0.28074) | -1 | -1 |
| G: -6322.94898 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.94924 HOMO: -6.41372 LUMO: 0.29388 factor:1 | 1 (-0.63457) | -1 | -1 |
| G: -6322.94898 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.73642 HOMO: -5.67902 LUMO: 1.77690 factor:1 | 1 (-0.42175) | -1 | -1 |
| G: -6322.94898 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.66611 HOMO: -6.55794 LUMO: 0.05170 factor:1 | 1 (-0.35144) | -1 | -1 |
| G: -6322.94898 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.60837 HOMO: -6.52801 LUMO: 0.25851 factor:1 | 1 (-0.29369) | -1 | -1 |
| G: -6322.94898 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.43944 HOMO: -7.08857 LUMO: 0.11157 factor:1 | 1 (-0.12476) | 1 | 1 |
| G: -6322.94898 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.51274 HOMO: -6.58243 LUMO: 0.75648 factor:1 | 1 (-0.19807) | -1 | -1 |
| G: -6322.94898 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.68897 HOMO: -7.22190 LUMO: 0.45171 factor:1 | 1 (-0.37429) | 1 | 1 |
| G: -6322.94898 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.72317 HOMO: -6.47087 LUMO: 0.00000 factor:1 | 1 (-0.40850) | -1 | -1 |
| G: -6322.94898 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.83591 HOMO: -6.78652 LUMO: 1.32247 factor:1 | 1 (-0.52123) | -1 | -1 |
| G: -6322.94898 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.56306 HOMO: -6.74026 LUMO: 1.45309 factor:1 | 1 (-0.24839) | -1 | -1 |
| G: -6322.94898 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.43650 HOMO: -6.69944 LUMO: 0.76464 factor:1 | 1 (-0.12183) | -1 | -1 |
| G: -6322.94898 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.40510 HOMO: -6.62325 LUMO: 0.64763 factor:1 | 1 (-0.09042) | -1 | -1 |
| G: -6322.94898 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.20942 HOMO: -6.45182 LUMO: 0.49253 factor:1 | -1 (0.10525) | -1 | -1 |
| G: -6322.94898 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.86867 HOMO: -7.14843 LUMO: 0.62586 factor:1 | 1 (-0.55400) | 1 | 1 |
| G: -6322.94898 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.75710 HOMO: -6.87087 LUMO: 1.53200 factor:1 | 1 (-0.44243) | -1 | -1 |
| G: -6322.94898 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.63536 HOMO: -6.54978 LUMO: 0.45171 factor:1 | 1 (-0.32069) | -1 | -1 |
| G: -6322.94898 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.64581 HOMO: -6.63686 LUMO: 0.80001 factor:1 | 1 (-0.33114) | -1 | -1 |
| G: -6322.94898 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.80742 HOMO: -7.00693 LUMO: 1.56193 factor:1 | 1 (-0.49274) | -1 | -1 |
| G: -6322.94898 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.69180 HOMO: -6.02460 LUMO: 1.72792 factor:1 | 1 (-0.37712) | -1 | -1 |
| G: -6322.94898 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.89811 HOMO: -6.36746 LUMO: -1.20002 factor:1 | 1 (-0.58344) | -1 | -1 |
| G: -6322.94898 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.84276 HOMO: -7.26816 LUMO: -1.06397 factor:1 | 1 (-0.52809) | 1 | 1 |
| G: -6322.94898 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.61158 HOMO: -7.34707 LUMO: -1.09662 factor:1 | 1 (-0.29690) | 1 | 1 |
| G: -6322.94898 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.52845 HOMO: -7.93212 LUMO: -0.13606 factor:1 | 1 (-0.21377) | 1 | 1 |
| G: -6322.94898 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.53468 HOMO: -6.80285 LUMO: 0.58504 factor:1 | 1 (-0.22000) | -1 | -1 |
| G: -6322.94898 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.42469 HOMO: -7.12938 LUMO: 0.32926 factor:1 | 1 (-0.11002) | 1 | -1 |
| G: -6322.94898 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.94908 HOMO: -6.86815 LUMO: -1.30070 factor:1 | 1 (-0.63441) | -1 | -1 |
| G: -6322.94898 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.71463 HOMO: -6.99333 LUMO: -1.03947 factor:1 | 1 (-0.39995) | -1 | -1 |
| G: -6322.94898 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.59819 HOMO: -7.56749 LUMO: -0.11157 factor:1 | 1 (-0.28352) | 1 | 1 |
| G: -6322.94898 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.76663 HOMO: -7.57293 LUMO: -0.07891 factor:1 | 1 (-0.45195) | 1 | 1 |
| G: -6322.94898 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.47653 HOMO: -7.30626 LUMO: 0.27211 factor:1 | 1 (-0.16185) | 1 | 1 |
| G: -6322.94898 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.49057 HOMO: -7.77974 LUMO: 0.27211 factor:1 | 1 (-0.17589) | 1 | 1 |
| G: -6322.94898 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.34504 HOMO: -7.11578 LUMO: 0.19864 factor:1 | 1 (-0.03037) | 1 | 1 |
| G: -6322.94898 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.61500 HOMO: -7.71171 LUMO: 0.57688 factor:1 | 1 (-0.30033) | 1 | 1 |
| G: -6322.94898 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.33919 HOMO: -7.83688 LUMO: 0.37824 factor:1 | 1 (-0.02452) | 1 | 1 |
| G: -6322.94898 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.33650 HOMO: -6.94979 LUMO: -1.66534 factor:1 | 1 (-0.02182) | -1 | -1 |
| G: -6322.94898 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.19353 HOMO: -6.97156 LUMO: -1.13199 factor:1 | -1 (0.12115) | -1 | -1 |
| G: -6322.94898 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.33541 HOMO: -6.91441 LUMO: -1.08301 factor:1 | 1 (-0.02074) | -1 | -1 |
| G: -6322.94898 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.20477 HOMO: -6.71849 LUMO: -0.74831 factor:1 | -1 (0.10991) | -1 | -1 |
| G: -6322.94898 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12586.96528 HOMO: -7.09401 LUMO: -1.77690 factor:1 | -1 (0.34939) | -1 | -1 |
| G: -6322.94898 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.44295 HOMO: -6.97156 LUMO: -1.45037 factor:1 | 1 (-0.12827) | -1 | -1 |
| G: -6322.94898 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.64031 HOMO: -7.22462 LUMO: -1.11295 factor:1 | 1 (-0.32564) | 1 | 1 |
| G: -6322.94898 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.83196 HOMO: -7.85321 LUMO: 0.16599 factor:1 | 1 (-0.51729) | 1 | 1 |
| G: -6322.94898 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.81838 HOMO: -7.71987 LUMO: 0.55511 factor:1 | 1 (-0.50371) | 1 | 1 |
| G: -6322.94898 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.61079 HOMO: -7.63551 LUMO: 0.14422 factor:1 | 1 (-0.29611) | 1 | 1 |
| G: -6322.94898 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.80676 HOMO: -6.98788 LUMO: -0.80546 factor:1 | 1 (-0.49209) | -1 | -1 |
| G: -6322.94898 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.81397 HOMO: -6.98788 LUMO: -1.16737 factor:1 | 1 (-0.49930) | -1 | -1 |
| G: -6322.94898 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.91980 HOMO: -6.56611 LUMO: -1.60819 factor:1 | 1 (-0.60513) | -1 | -1 |
| G: -6322.94898 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.69683 HOMO: -6.95251 LUMO: 0.66396 factor:1 | 1 (-0.38216) | -1 | -1 |
| G: -6322.94898 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.61838 HOMO: -7.35252 LUMO: 0.49797 factor:1 | 1 (-0.30371) | 1 | 1 |
| G: -6322.94898 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.60265 HOMO: -6.90897 LUMO: -0.81090 factor:1 | 1 (-0.28798) | -1 | -1 |
| G: -6322.94898 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.46610 HOMO: -7.04503 LUMO: -1.08301 factor:1 | 1 (-0.15143) | -1 | -1 |
| G: -6322.94898 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.39862 HOMO: -6.92530 LUMO: -1.29526 factor:1 | 1 (-0.08395) | -1 | -1 |
| G: -6322.94898 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.45351 HOMO: -6.93074 LUMO: -1.25444 factor:1 | 1 (-0.13883) | -1 | -1 |
| G: -6322.94898 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.47688 HOMO: -6.73482 LUMO: -0.62042 factor:1 | 1 (-0.16221) | -1 | -1 |
| G: -6322.94898 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.38599 HOMO: -7.67633 LUMO: 0.59593 factor:1 | 1 (-0.07132) | 1 | 1 |
| G: -6322.94898 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.67033 HOMO: -7.39061 LUMO: -0.19320 factor:1 | 1 (-0.35565) | 1 | 1 |
| G: -6322.94898 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.66442 HOMO: -7.55388 LUMO: -0.20136 factor:1 | 1 (-0.34975) | 1 | 1 |
| G: -6322.94898 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.67767 HOMO: -7.14027 LUMO: -0.99866 factor:1 | 1 (-0.36300) | 1 | 1 |
| G: -6322.94898 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.59743 HOMO: -6.75931 LUMO: -0.73199 factor:1 | 1 (-0.28275) | -1 | -1 |
| G: -6322.94898 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.35639 HOMO: -5.45044 LUMO: -0.18776 factor:1 | 1 (-0.04172) | -1 | -1 |
| G: -6322.94898 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.45541 HOMO: -6.70761 LUMO: -0.84083 factor:1 | 1 (-0.14074) | -1 | -1 |
| G: -6322.94898 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.39625 HOMO: -6.05453 LUMO: -1.06669 factor:1 | 1 (-0.08158) | -1 | -1 |
| G: -6322.94898 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.25522 HOMO: -6.86815 LUMO: -0.98233 factor:1 | -1 (0.05946) | -1 | -1 |
| G: -6322.94898 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.51952 HOMO: -6.73210 LUMO: -0.95240 factor:1 | 1 (-0.20485) | -1 | -1 |
| G: -6322.94898 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.83389 HOMO: -5.89671 LUMO: -1.05036 factor:1 | 1 (-0.51922) | -1 | -1 |
| G: -6322.94898 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.53892 HOMO: -7.61102 LUMO: 0.33470 factor:1 | 1 (-0.22425) | 1 | 1 |
| G: -6322.94898 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.59070 HOMO: -7.51034 LUMO: 0.23674 factor:1 | 1 (-0.27603) | 1 | 1 |
| G: -6322.94898 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.66608 HOMO: -7.41510 LUMO: 0.62858 factor:1 | 1 (-0.35141) | 1 | 1 |
| G: -6322.94898 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.74687 HOMO: -6.76203 LUMO: -1.72792 factor:1 | 1 (-0.43220) | -1 | -1 |
| G: -6322.94898 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.70246 HOMO: -6.60420 LUMO: -0.45715 factor:1 | 1 (-0.38779) | -1 | -1 |
| G: -6322.94898 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.38719 HOMO: -6.59060 LUMO: -0.58232 factor:1 | 1 (-0.07252) | -1 | -1 |
| G: -6322.94898 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.54673 HOMO: -7.43687 LUMO: -0.76736 factor:1 | 1 (-0.23206) | 1 | 1 |
| G: -6322.94898 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.38009 HOMO: -6.08719 LUMO: -0.48708 factor:1 | 1 (-0.06542) | -1 | -1 |
| G: -6322.94898 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.74995 HOMO: -5.88854 LUMO: -0.05714 factor:1 | 1 (-0.43527) | -1 | -1 |
| G: -6322.94898 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.69033 HOMO: -7.34435 LUMO: -0.71838 factor:1 | 1 (-0.37565) | 1 | 1 |
| G: -6322.94898 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.63841 HOMO: -7.46408 LUMO: -0.63130 factor:1 | 1 (-0.32373) | 1 | 1 |
| G: -6322.94898 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.36512 HOMO: -7.00965 LUMO: -1.24900 factor:1 | 1 (-0.05045) | -1 | -1 |
| G: -6322.94898 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.43827 HOMO: -6.91169 LUMO: -0.88981 factor:1 | 1 (-0.12359) | -1 | -1 |
| G: -6322.94898 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.30986 HOMO: -6.78652 LUMO: -0.82178 factor:1 | -1 (0.00482) | -1 | -1 |
| G: -6322.94898 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.19628 HOMO: -7.80423 LUMO: 0.87076 factor:1 | -1 (0.11840) | 1 | 1 |
| G: -6322.94898 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12586.98457 HOMO: -6.97700 LUMO: -1.00954 factor:1 | -1 (0.33010) | -1 | -1 |
| G: -6322.94898 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.52787 HOMO: -6.92530 LUMO: -0.88165 factor:1 | 1 (-0.21320) | -1 | -1 |
| G: -6322.94898 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.40319 HOMO: -7.14571 LUMO: -1.04492 factor:1 | 1 (-0.08852) | 1 | 1 |
| G: -6322.87766 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12588.02195 HOMO: -7.49674 LUMO: 0.34558 factor:1 | 1 (-0.77860) | 1 | 1 |
| G: -6322.87766 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12588.08797 HOMO: -6.44094 LUMO: -1.20819 factor:1 | 1 (-0.84461) | -1 | -1 |
| G: -6322.87766 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12588.15719 HOMO: -6.47359 LUMO: -1.14016 factor:1 | 1 (-0.91384) | -1 | -1 |
| G: -6322.87766 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.78918 HOMO: -6.61237 LUMO: -0.87076 factor:1 | 1 (-0.54583) | -1 | -1 |
| G: -6322.87766 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.85993 HOMO: -6.73754 LUMO: -1.09662 factor:1 | 1 (-0.61658) | -1 | -1 |
| G: -6322.87766 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.69441 HOMO: -6.97700 LUMO: 0.13061 factor:1 | 1 (-0.45106) | -1 | -1 |
| G: -6322.87766 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12588.07695 HOMO: -6.82734 LUMO: 0.59865 factor:1 | 1 (-0.83359) | -1 | -1 |
| G: -6322.87766 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12588.08105 HOMO: -6.86543 LUMO: -0.91430 factor:1 | 1 (-0.83770) | -1 | -1 |
| G: -6322.87766 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.76791 HOMO: -6.74298 LUMO: 0.28028 factor:1 | 1 (-0.52455) | -1 | -1 |
| G: -6322.87766 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.67101 HOMO: -6.75387 LUMO: 0.19592 factor:1 | 1 (-0.42765) | -1 | -1 |
| G: -6322.87766 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.88989 HOMO: -7.05591 LUMO: 0.10612 factor:1 | 1 (-0.64654) | -1 | -1 |
| G: -6322.87766 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.50722 HOMO: -6.86543 LUMO: 0.49253 factor:1 | 1 (-0.26387) | -1 | -1 |
| G: -6322.87766 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.67724 HOMO: -6.11440 LUMO: -1.12655 factor:1 | 1 (-0.43389) | -1 | -1 |
| G: -6322.87766 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.71941 HOMO: -6.77291 LUMO: -1.02859 factor:1 | 1 (-0.47606) | -1 | -1 |
| G: -6322.87766 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.84644 HOMO: -6.54978 LUMO: 0.29116 factor:1 | 1 (-0.60309) | -1 | -1 |
| G: -6322.87766 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.95455 HOMO: -7.18108 LUMO: 0.00000 factor:1 | 1 (-0.71120) | 1 | 1 |
| G: -6322.87766 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.61090 HOMO: -6.86271 LUMO: -1.15376 factor:1 | 1 (-0.36754) | -1 | -1 |
| G: -6322.87766 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.66499 HOMO: -6.78108 LUMO: -1.22723 factor:1 | 1 (-0.42164) | -1 | -1 |
| G: -6322.87766 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.86538 HOMO: -6.40828 LUMO: 0.02449 factor:1 | 1 (-0.62203) | -1 | -1 |
| G: -6322.87766 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.86747 HOMO: -6.43821 LUMO: 0.09796 factor:1 | 1 (-0.62412) | -1 | -1 |
| G: -6322.87766 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.76527 HOMO: -6.99877 LUMO: 0.40545 factor:1 | 1 (-0.52191) | -1 | -1 |
| G: -6322.87766 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12588.05330 HOMO: -6.68856 LUMO: 0.19320 factor:1 | 1 (-0.80995) | -1 | -1 |
| G: -6322.87766 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.67560 HOMO: -7.11034 LUMO: 0.31293 factor:1 | 1 (-0.43225) | 1 | 1 |
| G: -6322.87766 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.47318 HOMO: -6.92530 LUMO: -0.85444 factor:1 | 1 (-0.22983) | -1 | -1 |
| G: -6322.87766 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.61928 HOMO: -6.60148 LUMO: -0.59865 factor:1 | 1 (-0.37593) | -1 | -1 |
| G: -6322.87766 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.67305 HOMO: -6.72938 LUMO: 0.30749 factor:1 | 1 (-0.42969) | -1 | -1 |
| G: -6322.87766 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.66535 HOMO: -7.31170 LUMO: 0.06803 factor:1 | 1 (-0.42199) | 1 | 1 |
| G: -6322.87766 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.56717 HOMO: -7.09129 LUMO: -0.04626 factor:1 | 1 (-0.32382) | 1 | 1 |
| G: -6322.87766 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.44978 HOMO: -6.38379 LUMO: -0.76736 factor:1 | 1 (-0.20643) | -1 | -1 |
| G: -6322.87766 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.25987 HOMO: -6.13617 LUMO: -0.63947 factor:1 | 1 (-0.01652) | -1 | -1 |
| G: -6322.87766 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.42795 HOMO: -6.92258 LUMO: 0.37007 factor:1 | 1 (-0.18460) | -1 | -1 |
| G: -6322.87766 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12588.04734 HOMO: -6.35930 LUMO: 0.41361 factor:1 | 1 (-0.80399) | -1 | -1 |
| G: -6322.87766 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.75074 HOMO: -6.60420 LUMO: 0.26667 factor:1 | 1 (-0.50738) | -1 | -1 |
| G: -6322.87766 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.73574 HOMO: -6.04909 LUMO: 1.82588 factor:1 | 1 (-0.49239) | -1 | -1 |
| G: -6322.87766 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.98834 HOMO: -6.69672 LUMO: 1.72520 factor:1 | 1 (-0.74499) | -1 | -1 |
| G: -6322.87766 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.66102 HOMO: -6.50080 LUMO: 0.29116 factor:1 | 1 (-0.41767) | -1 | -1 |
| G: -6322.87766 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.83457 HOMO: -6.60692 LUMO: -0.43266 factor:1 | 1 (-0.59122) | -1 | -1 |
| G: -6322.87766 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.92976 HOMO: -6.93890 LUMO: 0.39729 factor:1 | 1 (-0.68641) | -1 | -1 |
| G: -6322.87766 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.78118 HOMO: -6.52801 LUMO: -0.47076 factor:1 | 1 (-0.53783) | -1 | -1 |
| G: -6322.87766 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.50357 HOMO: -6.41100 LUMO: 0.30477 factor:1 | 1 (-0.26022) | -1 | -1 |
| G: -6322.87766 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.41321 HOMO: -6.37291 LUMO: -0.80001 factor:1 | 1 (-0.16985) | -1 | -1 |
| G: -6322.87766 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.73063 HOMO: -6.51985 LUMO: 1.44765 factor:1 | 1 (-0.48727) | -1 | -1 |
| G: -6322.87766 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.59851 HOMO: -6.64774 LUMO: 0.04626 factor:1 | 1 (-0.35516) | -1 | -1 |
| G: -6322.87766 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.74622 HOMO: -6.65863 LUMO: 0.29933 factor:1 | 1 (-0.50287) | -1 | -1 |
| G: -6322.87766 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.70526 HOMO: -7.09673 LUMO: 0.28300 factor:1 | 1 (-0.46191) | 1 | 1 |
| G: -6322.87766 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.59541 HOMO: -6.57155 LUMO: -1.11567 factor:1 | 1 (-0.35206) | -1 | -1 |
| G: -6322.87766 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.94924 HOMO: -6.38379 LUMO: -0.60681 factor:1 | 1 (-0.70589) | -1 | -1 |
| G: -6322.87766 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.73642 HOMO: -6.60148 LUMO: 0.18232 factor:1 | 1 (-0.49307) | -1 | -1 |
| G: -6322.87766 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.66611 HOMO: -6.96067 LUMO: -0.52246 factor:1 | 1 (-0.42276) | -1 | -1 |
| G: -6322.87766 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.60837 HOMO: -6.57427 LUMO: -0.84627 factor:1 | 1 (-0.36501) | -1 | -1 |
| G: -6322.87766 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.43944 HOMO: -6.59332 LUMO: -0.98233 factor:1 | 1 (-0.19609) | -1 | -1 |
| G: -6322.87766 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.51274 HOMO: -6.20692 LUMO: -0.27483 factor:1 | 1 (-0.26939) | -1 | -1 |
| G: -6322.87766 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.68897 HOMO: -6.81373 LUMO: 0.74559 factor:1 | 1 (-0.44561) | -1 | -1 |
| G: -6322.87766 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.72317 HOMO: -6.60420 LUMO: 0.54695 factor:1 | 1 (-0.47982) | -1 | -1 |
| G: -6322.87766 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.83591 HOMO: -6.58788 LUMO: -0.31021 factor:1 | 1 (-0.59256) | -1 | -1 |
| G: -6322.87766 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.56306 HOMO: -6.72938 LUMO: 0.64763 factor:1 | 1 (-0.31971) | -1 | -1 |
| G: -6322.87766 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.43650 HOMO: -6.86815 LUMO: 0.32109 factor:1 | 1 (-0.19315) | -1 | -1 |
| G: -6322.87766 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.40510 HOMO: -6.63141 LUMO: 0.18776 factor:1 | 1 (-0.16174) | -1 | -1 |
| G: -6322.87766 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.20942 HOMO: -7.18653 LUMO: 0.09524 factor:1 | -1 (0.03393) | 1 | 1 |
| G: -6322.87766 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.86867 HOMO: -6.83550 LUMO: 0.03537 factor:1 | 1 (-0.62532) | -1 | -1 |
| G: -6322.87766 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.75710 HOMO: -7.47769 LUMO: 0.40817 factor:1 | 1 (-0.51375) | 1 | 1 |
| G: -6322.87766 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.63536 HOMO: -6.57971 LUMO: -0.63675 factor:1 | 1 (-0.39201) | -1 | -1 |
| G: -6322.87766 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.64581 HOMO: -6.74842 LUMO: -0.16327 factor:1 | 1 (-0.40246) | -1 | -1 |
| G: -6322.87766 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.80742 HOMO: -7.07224 LUMO: 0.61770 factor:1 | 1 (-0.56406) | 1 | 1 |
| G: -6322.87766 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.69180 HOMO: -6.83006 LUMO: 0.54695 factor:1 | 1 (-0.44844) | -1 | -1 |
| G: -6322.87766 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.89811 HOMO: -6.60148 LUMO: 1.23540 factor:1 | 1 (-0.65476) | -1 | -1 |
| G: -6322.87766 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.84276 HOMO: -6.99061 LUMO: 0.41089 factor:1 | 1 (-0.59941) | -1 | -1 |
| G: -6322.87766 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.61158 HOMO: -6.63686 LUMO: 0.85172 factor:1 | 1 (-0.36822) | -1 | -1 |
| G: -6322.87766 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.52845 HOMO: -6.50624 LUMO: 0.12517 factor:1 | 1 (-0.28509) | -1 | -1 |
| G: -6322.87766 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.53468 HOMO: -6.35658 LUMO: 0.36463 factor:1 | 1 (-0.29133) | -1 | -1 |
| G: -6322.87766 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.42469 HOMO: -6.34570 LUMO: 0.65035 factor:1 | 1 (-0.18134) | -1 | -1 |
| G: -6322.87766 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.94908 HOMO: -6.63141 LUMO: 1.25717 factor:1 | 1 (-0.70573) | -1 | -1 |
| G: -6322.87766 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.71463 HOMO: -6.91441 LUMO: 1.32792 factor:1 | 1 (-0.47127) | -1 | -1 |
| G: -6322.87766 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.59819 HOMO: -7.15387 LUMO: 0.64219 factor:1 | 1 (-0.35484) | 1 | 1 |
| G: -6322.87766 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.76663 HOMO: -7.17836 LUMO: 0.60409 factor:1 | 1 (-0.52327) | 1 | 1 |
| G: -6322.87766 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.47653 HOMO: -6.92258 LUMO: 0.49525 factor:1 | 1 (-0.23317) | -1 | -1 |
| G: -6322.87766 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.49057 HOMO: -6.31032 LUMO: 0.48708 factor:1 | 1 (-0.24722) | -1 | -1 |
| G: -6322.87766 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.34504 HOMO: -6.49808 LUMO: 0.31021 factor:1 | 1 (-0.10169) | -1 | -1 |
| G: -6322.87766 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.61500 HOMO: -6.48447 LUMO: 0.37552 factor:1 | 1 (-0.37165) | -1 | -1 |
| G: -6322.87766 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.33919 HOMO: -6.66135 LUMO: -1.08301 factor:1 | 1 (-0.09584) | -1 | -1 |
| G: -6322.87766 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.33650 HOMO: -6.33481 LUMO: -0.51974 factor:1 | 1 (-0.09314) | -1 | -1 |
| G: -6322.87766 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.19353 HOMO: -6.76475 LUMO: -0.15238 factor:1 | -1 (0.04982) | -1 | -1 |
| G: -6322.87766 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.33541 HOMO: -6.93346 LUMO: -0.10885 factor:1 | 1 (-0.09206) | -1 | -1 |
| G: -6322.87766 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.20477 HOMO: -7.19741 LUMO: 0.73199 factor:1 | -1 (0.03859) | 1 | 1 |
| G: -6322.87766 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12586.96528 HOMO: -6.82734 LUMO: 0.88437 factor:1 | -1 (0.27807) | -1 | -1 |
| G: -6322.87766 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.44295 HOMO: -7.01237 LUMO: 0.02721 factor:1 | 1 (-0.19960) | -1 | -1 |
| G: -6322.87766 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.64031 HOMO: -6.39195 LUMO: 1.46941 factor:1 | 1 (-0.39696) | -1 | -1 |
| G: -6322.87766 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.83196 HOMO: -6.53890 LUMO: 1.32792 factor:1 | 1 (-0.58861) | -1 | -1 |
| G: -6322.87766 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.81838 HOMO: -6.82734 LUMO: 1.98099 factor:1 | 1 (-0.57503) | -1 | -1 |
| G: -6322.87766 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.61079 HOMO: -6.74570 LUMO: 1.68983 factor:1 | 1 (-0.36744) | -1 | -1 |
| G: -6322.87766 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.80676 HOMO: -6.41100 LUMO: 1.39050 factor:1 | 1 (-0.56341) | -1 | -1 |
| G: -6322.87766 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.81397 HOMO: -5.92664 LUMO: 1.65989 factor:1 | 1 (-0.57062) | -1 | -1 |
| G: -6322.87766 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.91980 HOMO: -6.07630 LUMO: 1.54833 factor:1 | 1 (-0.67645) | -1 | -1 |
| G: -6322.87766 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.69683 HOMO: -6.45998 LUMO: 0.68573 factor:1 | 1 (-0.45348) | -1 | -1 |
| G: -6322.87766 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.61838 HOMO: -6.52801 LUMO: 0.41361 factor:1 | 1 (-0.37503) | -1 | -1 |
| G: -6322.87766 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.60265 HOMO: -6.77564 LUMO: 0.42178 factor:1 | 1 (-0.35930) | -1 | -1 |
| G: -6322.87766 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.46610 HOMO: -6.56339 LUMO: 1.65717 factor:1 | 1 (-0.22275) | -1 | -1 |
| G: -6322.87766 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.39862 HOMO: -5.85861 LUMO: 1.90752 factor:1 | 1 (-0.15527) | -1 | -1 |
| G: -6322.87766 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.45351 HOMO: -6.77019 LUMO: -2.48440 factor:1 | 1 (-0.21015) | -1 | -1 |
| G: -6322.87766 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.47688 HOMO: -6.53890 LUMO: -1.82588 factor:1 | 1 (-0.23353) | -1 | -1 |
| G: -6322.87766 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.38599 HOMO: -6.50352 LUMO: -1.66806 factor:1 | 1 (-0.14264) | -1 | -1 |
| G: -6322.87766 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.67033 HOMO: -6.90625 LUMO: 0.43538 factor:1 | 1 (-0.42697) | -1 | -1 |
| G: -6322.87766 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.66442 HOMO: -6.85455 LUMO: 0.53062 factor:1 | 1 (-0.42107) | -1 | -1 |
| G: -6322.87766 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.67767 HOMO: -6.49536 LUMO: 0.31021 factor:1 | 1 (-0.43432) | -1 | -1 |
| G: -6322.87766 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.59743 HOMO: -4.97696 LUMO: -0.09252 factor:1 | 1 (-0.35407) | -1 | -1 |
| G: -6322.87766 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.35639 HOMO: -5.31166 LUMO: 0.34286 factor:1 | 1 (-0.11304) | -1 | -1 |
| G: -6322.87766 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.45541 HOMO: -6.42461 LUMO: 0.74287 factor:1 | 1 (-0.21206) | -1 | -1 |
| G: -6322.87766 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.39625 HOMO: -6.59604 LUMO: 0.62858 factor:1 | 1 (-0.15290) | -1 | -1 |
| G: -6322.87766 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.25522 HOMO: -6.45998 LUMO: -0.61770 factor:1 | 1 (-0.01186) | -1 | -1 |
| G: -6322.87766 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.51952 HOMO: -6.75659 LUMO: -0.34014 factor:1 | 1 (-0.27617) | -1 | -1 |
| G: -6322.87766 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.83389 HOMO: -6.63958 LUMO: 0.36191 factor:1 | 1 (-0.59054) | -1 | -1 |
| G: -6322.87766 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.53892 HOMO: -5.92936 LUMO: -0.67484 factor:1 | 1 (-0.29557) | -1 | -1 |
| G: -6322.87766 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.59070 HOMO: -5.67630 LUMO: 1.80956 factor:1 | 1 (-0.34735) | -1 | -1 |
| G: -6322.87766 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.66608 HOMO: -6.50352 LUMO: -0.78369 factor:1 | 1 (-0.42273) | -1 | -1 |
| G: -6322.87766 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.74687 HOMO: -6.35930 LUMO: -0.75648 factor:1 | 1 (-0.50352) | -1 | -1 |
| G: -6322.87766 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.70246 HOMO: -6.74298 LUMO: 0.48980 factor:1 | 1 (-0.45911) | -1 | -1 |
| G: -6322.87766 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.38719 HOMO: -6.85183 LUMO: 0.15510 factor:1 | 1 (-0.14384) | -1 | -1 |
| G: -6322.87766 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.54673 HOMO: -6.90897 LUMO: 0.26123 factor:1 | 1 (-0.30338) | -1 | -1 |
| G: -6322.87766 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.38009 HOMO: -6.85999 LUMO: 0.47892 factor:1 | 1 (-0.13674) | -1 | -1 |
| G: -6322.87766 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.74995 HOMO: -6.69944 LUMO: 0.57416 factor:1 | 1 (-0.50659) | -1 | -1 |
| G: -6322.87766 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.69033 HOMO: -6.74026 LUMO: 0.69933 factor:1 | 1 (-0.44697) | -1 | -1 |
| G: -6322.87766 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.63841 HOMO: -6.52801 LUMO: 0.75376 factor:1 | 1 (-0.39505) | -1 | -1 |
| G: -6322.87766 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.36512 HOMO: -7.05863 LUMO: 0.44627 factor:1 | 1 (-0.12177) | -1 | -1 |
| G: -6322.87766 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.43827 HOMO: -6.96339 LUMO: 0.48164 factor:1 | 1 (-0.19492) | -1 | -1 |
| G: -6322.87766 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.30986 HOMO: -6.95795 LUMO: 0.44355 factor:1 | 1 (-0.06650) | -1 | -1 |
| G: -6322.87766 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.19628 HOMO: -6.36746 LUMO: 0.58777 factor:1 | -1 (0.04708) | -1 | -1 |
| G: -6322.87766 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12586.98457 HOMO: -6.69400 LUMO: 0.40545 factor:1 | -1 (0.25878) | -1 | -1 |
| G: -6322.87766 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.52787 HOMO: -6.30760 LUMO: -0.66668 factor:1 | 1 (-0.28452) | -1 | -1 |
| G: -6322.87766 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.40319 HOMO: -6.53617 LUMO: -0.64491 factor:1 | 1 (-0.15984) | -1 | -1 |
| G: -6322.82647 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12588.02195 HOMO: -6.80829 LUMO: 0.17415 factor:1 | 1 (-0.82978) | -1 | -1 |
| G: -6322.82647 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12588.08797 HOMO: -6.80285 LUMO: 0.73471 factor:1 | 1 (-0.89580) | -1 | -1 |
| G: -6322.82647 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12588.15719 HOMO: -6.43821 LUMO: 0.21769 factor:1 | 1 (-0.96502) | -1 | -1 |
| G: -6322.82647 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.78918 HOMO: -6.98788 LUMO: 0.10885 factor:1 | 1 (-0.59702) | -1 | -1 |
| G: -6322.82647 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.85993 HOMO: -7.15115 LUMO: 0.40817 factor:1 | 1 (-0.66777) | 1 | 1 |
| G: -6322.82647 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.69441 HOMO: -6.00011 LUMO: -0.98505 factor:1 | 1 (-0.50224) | -1 | -1 |
| G: -6322.82647 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12588.07695 HOMO: -6.16882 LUMO: -0.77825 factor:1 | 1 (-0.88478) | -1 | -1 |
| G: -6322.82647 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12588.08105 HOMO: -6.30760 LUMO: 0.34831 factor:1 | 1 (-0.88889) | -1 | -1 |
| G: -6322.82647 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.76791 HOMO: -6.64502 LUMO: 0.63403 factor:1 | 1 (-0.57574) | -1 | -1 |
| G: -6322.82647 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.67101 HOMO: -6.93618 LUMO: 0.96600 factor:1 | 1 (-0.47884) | -1 | -1 |
| G: -6322.82647 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.88989 HOMO: -6.45182 LUMO: 0.16327 factor:1 | 1 (-0.69773) | -1 | -1 |
| G: -6322.82647 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.50722 HOMO: -6.99605 LUMO: 0.20953 factor:1 | 1 (-0.31505) | -1 | -1 |
| G: -6322.82647 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.67724 HOMO: -6.72665 LUMO: 0.32654 factor:1 | 1 (-0.48507) | -1 | -1 |
| G: -6322.82647 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.71941 HOMO: -6.38379 LUMO: 0.45443 factor:1 | 1 (-0.52725) | -1 | -1 |
| G: -6322.82647 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.84644 HOMO: -6.65318 LUMO: 0.04354 factor:1 | 1 (-0.65427) | -1 | -1 |
| G: -6322.82647 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.95455 HOMO: -6.94707 LUMO: -1.68438 factor:1 | 1 (-0.76238) | -1 | -1 |
| G: -6322.82647 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.61090 HOMO: -6.71849 LUMO: 0.15783 factor:1 | 1 (-0.41873) | -1 | -1 |
| G: -6322.82647 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.66499 HOMO: -6.97156 LUMO: 0.43266 factor:1 | 1 (-0.47283) | -1 | -1 |
| G: -6322.82647 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.86538 HOMO: -6.91441 LUMO: -0.54695 factor:1 | 1 (-0.67321) | -1 | -1 |
| G: -6322.82647 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.86747 HOMO: -6.74842 LUMO: -0.76192 factor:1 | 1 (-0.67530) | -1 | -1 |
| G: -6322.82647 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.76527 HOMO: -6.70489 LUMO: 0.19048 factor:1 | 1 (-0.57310) | -1 | -1 |
| G: -6322.82647 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12588.05330 HOMO: -7.25728 LUMO: 0.33470 factor:1 | 1 (-0.86113) | 1 | -1 |
| G: -6322.82647 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.67560 HOMO: -6.96339 LUMO: 0.55511 factor:1 | 1 (-0.48344) | -1 | -1 |
| G: -6322.82647 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.47318 HOMO: -6.77564 LUMO: 0.72382 factor:1 | 1 (-0.28101) | -1 | -1 |
| G: -6322.82647 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.61928 HOMO: -6.75387 LUMO: 0.39729 factor:1 | 1 (-0.42711) | -1 | -1 |
| G: -6322.82647 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.67305 HOMO: -7.00149 LUMO: 0.06531 factor:1 | 1 (-0.48088) | -1 | -1 |
| G: -6322.82647 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.66535 HOMO: -7.09945 LUMO: 0.33470 factor:1 | 1 (-0.47318) | 1 | 1 |
| G: -6322.82647 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.56717 HOMO: -7.20830 LUMO: 0.59593 factor:1 | 1 (-0.37500) | 1 | 1 |
| G: -6322.82647 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.44978 HOMO: -6.40556 LUMO: 0.56600 factor:1 | 1 (-0.25761) | -1 | -1 |
| G: -6322.82647 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.25987 HOMO: -6.77291 LUMO: 0.73471 factor:1 | 1 (-0.06770) | -1 | -1 |
| G: -6322.82647 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.42795 HOMO: -6.65046 LUMO: 0.09796 factor:1 | 1 (-0.23579) | -1 | -1 |
| G: -6322.82647 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12588.04734 HOMO: -6.95795 LUMO: 0.22313 factor:1 | 1 (-0.85517) | -1 | -1 |
| G: -6322.82647 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.75074 HOMO: -6.85727 LUMO: 0.04626 factor:1 | 1 (-0.55857) | -1 | -1 |
| G: -6322.82647 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.73574 HOMO: -7.27360 LUMO: 0.42178 factor:1 | 1 (-0.54357) | 1 | 1 |
| G: -6322.82647 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.98834 HOMO: -6.78924 LUMO: -0.13334 factor:1 | 1 (-0.79618) | -1 | -1 |
| G: -6322.82647 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.66102 HOMO: -6.63141 LUMO: 0.38368 factor:1 | 1 (-0.46885) | -1 | -1 |
| G: -6322.82647 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.83457 HOMO: -6.92258 LUMO: 0.39184 factor:1 | 1 (-0.64241) | -1 | -1 |
| G: -6322.82647 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.92976 HOMO: -6.19331 LUMO: -0.46804 factor:1 | 1 (-0.73759) | -1 | -1 |
| G: -6322.82647 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.78118 HOMO: -7.26544 LUMO: -0.05442 factor:1 | 1 (-0.58902) | 1 | 1 |
| G: -6322.82647 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.50357 HOMO: -7.09401 LUMO: 0.30749 factor:1 | 1 (-0.31141) | 1 | 1 |
| G: -6322.82647 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.41321 HOMO: -6.14705 LUMO: -0.88709 factor:1 | 1 (-0.22104) | -1 | -1 |
| G: -6322.82647 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.73063 HOMO: -6.53617 LUMO: -0.28572 factor:1 | 1 (-0.53846) | -1 | -1 |
| G: -6322.82647 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.59851 HOMO: -6.37291 LUMO: -0.67212 factor:1 | 1 (-0.40635) | -1 | -1 |
| G: -6322.82647 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.74622 HOMO: -6.65591 LUMO: 0.03810 factor:1 | 1 (-0.55405) | -1 | -1 |
| G: -6322.82647 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.70526 HOMO: -7.11034 LUMO: 0.75103 factor:1 | 1 (-0.51310) | 1 | 1 |
| G: -6322.82647 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.59541 HOMO: -6.85183 LUMO: -0.05987 factor:1 | 1 (-0.40325) | -1 | -1 |
| G: -6322.82647 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.94924 HOMO: -6.70761 LUMO: -0.05442 factor:1 | 1 (-0.75708) | -1 | -1 |
| G: -6322.82647 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.73642 HOMO: -6.23413 LUMO: 0.06259 factor:1 | 1 (-0.54425) | -1 | -1 |
| G: -6322.82647 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.66611 HOMO: -6.55794 LUMO: 0.74015 factor:1 | 1 (-0.47394) | -1 | -1 |
| G: -6322.82647 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.60837 HOMO: -7.27905 LUMO: 0.26939 factor:1 | 1 (-0.41620) | 1 | 1 |
| G: -6322.82647 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.43944 HOMO: -6.34842 LUMO: -0.86804 factor:1 | 1 (-0.24727) | -1 | -1 |
| G: -6322.82647 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.51274 HOMO: -6.27222 LUMO: 1.46125 factor:1 | 1 (-0.32058) | -1 | -1 |
| G: -6322.82647 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.68897 HOMO: -6.65046 LUMO: 2.04902 factor:1 | 1 (-0.49680) | -1 | -1 |
| G: -6322.82647 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.72317 HOMO: -7.11850 LUMO: -1.14016 factor:1 | 1 (-0.53100) | 1 | -1 |
| G: -6322.82647 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.83591 HOMO: -6.88720 LUMO: -1.20274 factor:1 | 1 (-0.64374) | -1 | -1 |
| G: -6322.82647 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.56306 HOMO: -6.69400 LUMO: -0.31565 factor:1 | 1 (-0.37089) | -1 | -1 |
| G: -6322.82647 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.43650 HOMO: -6.95523 LUMO: -1.55377 factor:1 | 1 (-0.24433) | -1 | -1 |
| G: -6322.82647 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.40510 HOMO: -6.41372 LUMO: -0.83539 factor:1 | 1 (-0.21293) | -1 | -1 |
| G: -6322.82647 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.20942 HOMO: -6.13889 LUMO: -0.90070 factor:1 | 1 (-0.01725) | -1 | -1 |
| G: -6322.82647 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.86867 HOMO: -6.44366 LUMO: -0.55511 factor:1 | 1 (-0.67650) | -1 | -1 |
| G: -6322.82647 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.75710 HOMO: -6.10079 LUMO: -0.71022 factor:1 | 1 (-0.56494) | -1 | -1 |
| G: -6322.82647 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.63536 HOMO: -6.90353 LUMO: -0.64763 factor:1 | 1 (-0.44319) | -1 | -1 |
| G: -6322.82647 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.64581 HOMO: -6.65046 LUMO: -0.82450 factor:1 | 1 (-0.45364) | -1 | -1 |
| G: -6322.82647 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.80742 HOMO: -6.81645 LUMO: -0.85444 factor:1 | 1 (-0.61525) | -1 | -1 |
| G: -6322.82647 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.69180 HOMO: -6.20692 LUMO: 1.30887 factor:1 | 1 (-0.49963) | -1 | -1 |
| G: -6322.82647 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.89811 HOMO: -5.96201 LUMO: 1.33880 factor:1 | 1 (-0.70594) | -1 | -1 |
| G: -6322.82647 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.84276 HOMO: -6.52529 LUMO: 1.58914 factor:1 | 1 (-0.65060) | -1 | -1 |
| G: -6322.82647 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.61158 HOMO: -6.58516 LUMO: 1.97555 factor:1 | 1 (-0.41941) | -1 | -1 |
| G: -6322.82647 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.52845 HOMO: -6.84366 LUMO: 0.15783 factor:1 | 1 (-0.33628) | -1 | -1 |
| G: -6322.82647 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.53468 HOMO: -6.45726 LUMO: 0.42994 factor:1 | 1 (-0.34251) | -1 | -1 |
| G: -6322.82647 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.42469 HOMO: -6.75387 LUMO: 0.14422 factor:1 | 1 (-0.23252) | -1 | -1 |
| G: -6322.82647 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.94908 HOMO: -6.69944 LUMO: 1.79051 factor:1 | 1 (-0.75691) | -1 | -1 |
| G: -6322.82647 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.71463 HOMO: -6.59876 LUMO: 1.90208 factor:1 | 1 (-0.52246) | -1 | -1 |
| G: -6322.82647 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.59819 HOMO: -7.05863 LUMO: 1.20819 factor:1 | 1 (-0.40602) | -1 | -1 |
| G: -6322.82647 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.76663 HOMO: -6.54978 LUMO: 2.01636 factor:1 | 1 (-0.57446) | -1 | -1 |
| G: -6322.82647 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.47653 HOMO: -5.52119 LUMO: 1.95106 factor:1 | 1 (-0.28436) | -1 | -1 |
| G: -6322.82647 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.49057 HOMO: -6.53617 LUMO: 1.60275 factor:1 | 1 (-0.29840) | -1 | -1 |
| G: -6322.82647 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.34504 HOMO: -6.11440 LUMO: 1.89119 factor:1 | 1 (-0.15287) | -1 | -1 |
| G: -6322.82647 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.61500 HOMO: -7.31986 LUMO: 0.48708 factor:1 | 1 (-0.42284) | 1 | 1 |
| G: -6322.82647 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.33919 HOMO: -6.76475 LUMO: -0.75648 factor:1 | 1 (-0.14702) | -1 | -1 |
| G: -6322.82647 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.33650 HOMO: -6.76747 LUMO: -1.06941 factor:1 | 1 (-0.14433) | -1 | -1 |
| G: -6322.82647 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.19353 HOMO: -6.87087 LUMO: 0.72927 factor:1 | 1 (-0.00136) | -1 | -1 |
| G: -6322.82647 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.33541 HOMO: -7.00965 LUMO: 0.02177 factor:1 | 1 (-0.14324) | -1 | -1 |
| G: -6322.82647 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.20477 HOMO: -6.54706 LUMO: -0.03265 factor:1 | 1 (-0.01260) | -1 | -1 |
| G: -6322.82647 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12586.96528 HOMO: -6.62325 LUMO: -0.63675 factor:1 | -1 (0.22689) | -1 | -1 |
| G: -6322.82647 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.44295 HOMO: -7.03414 LUMO: -1.24084 factor:1 | 1 (-0.25078) | -1 | -1 |
| G: -6322.82647 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.64031 HOMO: -7.04503 LUMO: -0.10068 factor:1 | 1 (-0.44814) | -1 | -1 |
| G: -6322.82647 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.83196 HOMO: -6.67223 LUMO: 0.03537 factor:1 | 1 (-0.63979) | -1 | -1 |
| G: -6322.82647 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.81838 HOMO: -6.82734 LUMO: 0.58777 factor:1 | 1 (-0.62622) | -1 | -1 |
| G: -6322.82647 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.61079 HOMO: -6.84366 LUMO: 0.46531 factor:1 | 1 (-0.41862) | -1 | -1 |
| G: -6322.82647 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.80676 HOMO: -7.03959 LUMO: -1.15104 factor:1 | 1 (-0.61460) | -1 | -1 |
| G: -6322.82647 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.81397 HOMO: -6.91169 LUMO: -0.41361 factor:1 | 1 (-0.62181) | -1 | -1 |
| G: -6322.82647 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.91980 HOMO: -7.10217 LUMO: -0.44627 factor:1 | 1 (-0.72763) | 1 | 1 |
| G: -6322.82647 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.69683 HOMO: -6.88176 LUMO: -0.19592 factor:1 | 1 (-0.50466) | -1 | -1 |
| G: -6322.82647 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.61838 HOMO: -7.21374 LUMO: -0.46531 factor:1 | 1 (-0.42621) | 1 | 1 |
| G: -6322.82647 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.60265 HOMO: -6.54978 LUMO: 0.16871 factor:1 | 1 (-0.41048) | -1 | -1 |
| G: -6322.82647 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.46610 HOMO: -6.71305 LUMO: -0.13061 factor:1 | 1 (-0.27394) | -1 | -1 |
| G: -6322.82647 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.39862 HOMO: -6.74842 LUMO: -0.36191 factor:1 | 1 (-0.20645) | -1 | -1 |
| G: -6322.82647 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.45351 HOMO: -6.74570 LUMO: -0.09796 factor:1 | 1 (-0.26134) | -1 | -1 |
| G: -6322.82647 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.47688 HOMO: -6.93890 LUMO: -0.27211 factor:1 | 1 (-0.28471) | -1 | -1 |
| G: -6322.82647 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.38599 HOMO: -6.88720 LUMO: -0.18776 factor:1 | 1 (-0.19383) | -1 | -1 |
| G: -6322.82647 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.67033 HOMO: -6.74842 LUMO: 0.02993 factor:1 | 1 (-0.47816) | -1 | -1 |
| G: -6322.82647 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.66442 HOMO: -6.70216 LUMO: 0.01361 factor:1 | 1 (-0.47225) | -1 | -1 |
| G: -6322.82647 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.67767 HOMO: -6.90625 LUMO: 0.00544 factor:1 | 1 (-0.48551) | -1 | -1 |
| G: -6322.82647 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.59743 HOMO: -6.18243 LUMO: 0.25851 factor:1 | 1 (-0.40526) | -1 | -1 |
| G: -6322.82647 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.35639 HOMO: -6.32937 LUMO: -0.20953 factor:1 | 1 (-0.16422) | -1 | -1 |
| G: -6322.82647 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.45541 HOMO: -6.78108 LUMO: 0.00544 factor:1 | 1 (-0.26324) | -1 | -1 |
| G: -6322.82647 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.39625 HOMO: -5.97562 LUMO: 0.28572 factor:1 | 1 (-0.20409) | -1 | -1 |
| G: -6322.82647 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.25522 HOMO: -5.97290 LUMO: -0.18504 factor:1 | 1 (-0.06305) | -1 | -1 |
| G: -6322.82647 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.51952 HOMO: -6.12800 LUMO: 0.42178 factor:1 | 1 (-0.32735) | -1 | -1 |
| G: -6322.82647 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.83389 HOMO: -6.24229 LUMO: -0.00816 factor:1 | 1 (-0.64173) | -1 | -1 |
| G: -6322.82647 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.53892 HOMO: -6.61781 LUMO: 0.12789 factor:1 | 1 (-0.34675) | -1 | -1 |
| G: -6322.82647 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.59070 HOMO: -6.70489 LUMO: 0.14694 factor:1 | 1 (-0.39854) | -1 | -1 |
| G: -6322.82647 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.66608 HOMO: -6.86543 LUMO: -0.21225 factor:1 | 1 (-0.47391) | -1 | -1 |
| G: -6322.82647 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.74687 HOMO: -6.90081 LUMO: -0.20136 factor:1 | 1 (-0.55470) | -1 | -1 |
| G: -6322.82647 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.70246 HOMO: -7.12938 LUMO: -0.25851 factor:1 | 1 (-0.51030) | 1 | 1 |
| G: -6322.82647 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.38719 HOMO: -6.93074 LUMO: -0.26667 factor:1 | 1 (-0.19502) | -1 | -1 |
| G: -6322.82647 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.54673 HOMO: -7.00421 LUMO: -0.31021 factor:1 | 1 (-0.35456) | -1 | -1 |
| G: -6322.82647 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.38009 HOMO: -7.10761 LUMO: -0.17415 factor:1 | 1 (-0.18792) | 1 | 1 |
| G: -6322.82647 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.74995 HOMO: -8.21240 LUMO: 0.05987 factor:1 | 1 (-0.55778) | 1 | 1 |
| G: -6322.82647 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.69033 HOMO: -7.14843 LUMO: -0.46531 factor:1 | 1 (-0.49816) | 1 | -1 |
| G: -6322.82647 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.63841 HOMO: -6.80829 LUMO: -0.29933 factor:1 | 1 (-0.44624) | -1 | -1 |
| G: -6322.82647 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.36512 HOMO: -6.84094 LUMO: -0.53606 factor:1 | 1 (-0.17296) | -1 | -1 |
| G: -6322.82647 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.43827 HOMO: -6.81917 LUMO: -0.26667 factor:1 | 1 (-0.24610) | -1 | -1 |
| G: -6322.82647 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.30986 HOMO: -6.85727 LUMO: -1.20002 factor:1 | 1 (-0.11769) | -1 | -1 |
| G: -6322.82647 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.19628 HOMO: -6.39468 LUMO: -1.06941 factor:1 | 1 (-0.00411) | -1 | -1 |
| G: -6322.82647 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12586.98457 HOMO: -6.00827 LUMO: -1.94017 factor:1 | -1 (0.20760) | -1 | -1 |
| G: -6322.82647 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.52787 HOMO: -6.80829 LUMO: 0.18504 factor:1 | 1 (-0.33571) | -1 | -1 |
| G: -6322.82647 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.40319 HOMO: -6.54434 LUMO: -0.95784 factor:1 | 1 (-0.21102) | -1 | -1 |
| G: -6322.69006 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12588.02195 HOMO: -6.45454 LUMO: -0.07347 factor:1 | 1 (-0.96619) | -1 | -1 |
| G: -6322.69006 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12588.08797 HOMO: -5.33887 LUMO: 1.11839 factor:1 | 1 (-1.03221) | -1 | -1 |
| G: -6322.69006 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12588.15719 HOMO: -5.75249 LUMO: 0.70477 factor:1 | 1 (-1.10144) | -1 | -1 |
| G: -6322.69006 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.78918 HOMO: -5.64092 LUMO: 0.87076 factor:1 | 1 (-0.73343) | -1 | -1 |
| G: -6322.69006 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.85993 HOMO: -5.14295 LUMO: 1.06124 factor:1 | 1 (-0.80418) | -1 | -1 |
| G: -6322.69006 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.69441 HOMO: -5.05043 LUMO: 1.21091 factor:1 | 1 (-0.63865) | -1 | -1 |
| G: -6322.69006 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12588.07695 HOMO: -5.05588 LUMO: 1.02859 factor:1 | 1 (-1.02119) | -1 | -1 |
| G: -6322.69006 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12588.08105 HOMO: -5.76337 LUMO: 0.79457 factor:1 | 1 (-1.02530) | -1 | -1 |
| G: -6322.69006 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.76791 HOMO: -5.01506 LUMO: 1.00138 factor:1 | 1 (-0.71215) | -1 | -1 |
| G: -6322.69006 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.67101 HOMO: -4.84363 LUMO: 1.53744 factor:1 | 1 (-0.61525) | -1 | -1 |
| G: -6322.69006 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.88989 HOMO: -5.17833 LUMO: 1.45309 factor:1 | 1 (-0.83414) | -1 | -1 |
| G: -6322.69006 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.50722 HOMO: -5.13751 LUMO: 0.51157 factor:1 | 1 (-0.45146) | -1 | -1 |
| G: -6322.69006 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.67724 HOMO: -5.56473 LUMO: 0.32109 factor:1 | 1 (-0.62148) | -1 | -1 |
| G: -6322.69006 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.71941 HOMO: -4.69941 LUMO: 1.14016 factor:1 | 1 (-0.66366) | -1 | -1 |
| G: -6322.69006 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.84644 HOMO: -4.49260 LUMO: 1.86398 factor:1 | 1 (-0.79068) | -1 | -1 |
| G: -6322.69006 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.95455 HOMO: -4.32117 LUMO: 1.68438 factor:1 | 1 (-0.89879) | -1 | -1 |
| G: -6322.69006 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.61090 HOMO: -4.44906 LUMO: 1.37690 factor:1 | 1 (-0.55514) | -1 | -1 |
| G: -6322.69006 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.66499 HOMO: -4.62049 LUMO: 1.34968 factor:1 | 1 (-0.60924) | -1 | -1 |
| G: -6322.69006 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.86538 HOMO: -4.59600 LUMO: 1.58370 factor:1 | 1 (-0.80962) | -1 | -1 |
| G: -6322.69006 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.86747 HOMO: -4.98785 LUMO: 1.46669 factor:1 | 1 (-0.81172) | -1 | -1 |
| G: -6322.69006 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.76527 HOMO: -5.06676 LUMO: 1.27349 factor:1 | 1 (-0.70951) | -1 | -1 |
| G: -6322.69006 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12588.05330 HOMO: -5.09125 LUMO: 1.13471 factor:1 | 1 (-0.99754) | -1 | -1 |
| G: -6322.69006 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.67560 HOMO: -4.84635 LUMO: 1.33608 factor:1 | 1 (-0.61985) | -1 | -1 |
| G: -6322.69006 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.47318 HOMO: -4.94431 LUMO: 1.18370 factor:1 | 1 (-0.41742) | -1 | -1 |
| G: -6322.69006 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.61928 HOMO: -4.92526 LUMO: 1.39867 factor:1 | 1 (-0.56352) | -1 | -1 |
| G: -6322.69006 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.67305 HOMO: -5.71983 LUMO: 0.60137 factor:1 | 1 (-0.61729) | -1 | -1 |
| G: -6322.69006 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.66535 HOMO: -5.10486 LUMO: 1.05580 factor:1 | 1 (-0.60959) | -1 | -1 |
| G: -6322.69006 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.56717 HOMO: -5.20282 LUMO: 1.01226 factor:1 | 1 (-0.51141) | -1 | -1 |
| G: -6322.69006 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.44978 HOMO: -4.98513 LUMO: 1.53744 factor:1 | 1 (-0.39402) | -1 | -1 |
| G: -6322.69006 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.25987 HOMO: -5.67085 LUMO: 0.17687 factor:1 | 1 (-0.20411) | -1 | -1 |
| G: -6322.69006 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.42795 HOMO: -5.87222 LUMO: 0.12517 factor:1 | 1 (-0.37220) | -1 | -1 |
| G: -6322.69006 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12588.04734 HOMO: -5.20826 LUMO: 0.91702 factor:1 | 1 (-0.99158) | -1 | -1 |
| G: -6322.69006 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.75074 HOMO: -5.94569 LUMO: 0.63130 factor:1 | 1 (-0.69498) | -1 | -1 |
| G: -6322.69006 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.73574 HOMO: -5.35792 LUMO: 0.91430 factor:1 | 1 (-0.67999) | -1 | -1 |
| G: -6322.69006 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.98834 HOMO: -5.36336 LUMO: 1.44220 factor:1 | 1 (-0.93259) | -1 | -1 |
| G: -6322.69006 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.66102 HOMO: -5.83412 LUMO: 0.71294 factor:1 | 1 (-0.60526) | -1 | -1 |
| G: -6322.69006 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.83457 HOMO: -4.97696 LUMO: 1.72792 factor:1 | 1 (-0.77882) | -1 | -1 |
| G: -6322.69006 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.92976 HOMO: -5.55929 LUMO: 0.23130 factor:1 | 1 (-0.87400) | -1 | -1 |
| G: -6322.69006 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.78118 HOMO: -5.71167 LUMO: 0.47348 factor:1 | 1 (-0.72543) | -1 | -1 |
| G: -6322.69006 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.50357 HOMO: -7.31986 LUMO: -2.54699 factor:1 | 1 (-0.44782) | -1 | -1 |
| G: -6322.69006 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.41321 HOMO: -5.34704 LUMO: 1.19730 factor:1 | 1 (-0.35745) | -1 | -1 |
| G: -6322.69006 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.73063 HOMO: -5.45860 LUMO: 0.80818 factor:1 | 1 (-0.67487) | -1 | -1 |
| G: -6322.69006 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.59851 HOMO: -5.12663 LUMO: 1.20274 factor:1 | 1 (-0.54276) | -1 | -1 |
| G: -6322.69006 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.74622 HOMO: -5.37153 LUMO: 1.05580 factor:1 | 1 (-0.69046) | -1 | -1 |
| G: -6322.69006 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.70526 HOMO: -5.47221 LUMO: 0.97961 factor:1 | 1 (-0.64951) | -1 | -1 |
| G: -6322.69006 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.59541 HOMO: -5.06948 LUMO: 1.12111 factor:1 | 1 (-0.53966) | -1 | -1 |
| G: -6322.69006 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.94924 HOMO: -5.19737 LUMO: 1.25444 factor:1 | 1 (-0.89349) | -1 | -1 |
| G: -6322.69006 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.73642 HOMO: -5.27901 LUMO: 1.00682 factor:1 | 1 (-0.68067) | -1 | -1 |
| G: -6322.69006 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.66611 HOMO: -5.38513 LUMO: 0.49253 factor:1 | 1 (-0.61035) | -1 | -1 |
| G: -6322.69006 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.60837 HOMO: -5.12390 LUMO: 1.22995 factor:1 | 1 (-0.55261) | -1 | -1 |
| G: -6322.69006 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.43944 HOMO: -5.31438 LUMO: 0.70205 factor:1 | 1 (-0.38368) | -1 | -1 |
| G: -6322.69006 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.51274 HOMO: -5.17561 LUMO: 1.04492 factor:1 | 1 (-0.45699) | -1 | -1 |
| G: -6322.69006 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.68897 HOMO: -4.94431 LUMO: 1.52656 factor:1 | 1 (-0.63321) | -1 | -1 |
| G: -6322.69006 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.72317 HOMO: -5.13751 LUMO: 0.93879 factor:1 | 1 (-0.66741) | -1 | -1 |
| G: -6322.69006 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.83591 HOMO: -5.49942 LUMO: 0.97689 factor:1 | 1 (-0.78015) | -1 | -1 |
| G: -6322.69006 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.56306 HOMO: -5.79058 LUMO: 0.53879 factor:1 | 1 (-0.50730) | -1 | -1 |
| G: -6322.69006 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.43650 HOMO: -5.36881 LUMO: 1.56465 factor:1 | 1 (-0.38074) | -1 | -1 |
| G: -6322.69006 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.40510 HOMO: -4.67492 LUMO: 1.32792 factor:1 | 1 (-0.34934) | -1 | -1 |
| G: -6322.69006 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.20942 HOMO: -4.60145 LUMO: 1.19458 factor:1 | 1 (-0.15366) | -1 | -1 |
| G: -6322.69006 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.86867 HOMO: -4.49260 LUMO: 1.60547 factor:1 | 1 (-0.81291) | -1 | -1 |
| G: -6322.69006 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.75710 HOMO: -4.65043 LUMO: 1.34696 factor:1 | 1 (-0.70135) | -1 | -1 |
| G: -6322.69006 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.63536 HOMO: -4.77560 LUMO: 1.35241 factor:1 | 1 (-0.57960) | -1 | -1 |
| G: -6322.69006 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.64581 HOMO: -4.94431 LUMO: 1.17825 factor:1 | 1 (-0.59005) | -1 | -1 |
| G: -6322.69006 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.80742 HOMO: -4.87084 LUMO: 1.41771 factor:1 | 1 (-0.75166) | -1 | -1 |
| G: -6322.69006 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.69180 HOMO: -5.34432 LUMO: 1.16737 factor:1 | 1 (-0.63604) | -1 | -1 |
| G: -6322.69006 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.89811 HOMO: -4.94975 LUMO: 1.67622 factor:1 | 1 (-0.84236) | -1 | -1 |
| G: -6322.69006 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.84276 HOMO: -4.81369 LUMO: 1.14288 factor:1 | 1 (-0.78701) | -1 | -1 |
| G: -6322.69006 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.61158 HOMO: -5.22459 LUMO: 0.29660 factor:1 | 1 (-0.55582) | -1 | -1 |
| G: -6322.69006 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.52845 HOMO: -5.21642 LUMO: 0.37824 factor:1 | 1 (-0.47269) | -1 | -1 |
| G: -6322.69006 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.53468 HOMO: -5.00417 LUMO: 1.01226 factor:1 | 1 (-0.47892) | -1 | -1 |
| G: -6322.69006 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.42469 HOMO: -5.46677 LUMO: 0.10612 factor:1 | 1 (-0.36893) | -1 | -1 |
| G: -6322.69006 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.94908 HOMO: -5.51303 LUMO: 0.54151 factor:1 | 1 (-0.89332) | -1 | -1 |
| G: -6322.69006 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.71463 HOMO: -5.63004 LUMO: 0.17960 factor:1 | 1 (-0.65887) | -1 | -1 |
| G: -6322.69006 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.59819 HOMO: -4.79193 LUMO: 1.12111 factor:1 | 1 (-0.54243) | -1 | -1 |
| G: -6322.69006 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.76663 HOMO: -5.43411 LUMO: 0.45987 factor:1 | 1 (-0.71087) | -1 | -1 |
| G: -6322.69006 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.47653 HOMO: -7.06135 LUMO: -2.13881 factor:1 | 1 (-0.42077) | 1 | 1 |
| G: -6322.69006 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.49057 HOMO: -5.33071 LUMO: 1.14016 factor:1 | 1 (-0.43481) | -1 | -1 |
| G: -6322.69006 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.34504 HOMO: -7.12394 LUMO: -0.03810 factor:1 | 1 (-0.28928) | 1 | 1 |
| G: -6322.69006 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.61500 HOMO: -7.20558 LUMO: -2.50889 factor:1 | 1 (-0.55925) | 1 | 1 |
| G: -6322.69006 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.33919 HOMO: -7.26816 LUMO: -2.11432 factor:1 | 1 (-0.28343) | 1 | 1 |
| G: -6322.69006 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.33650 HOMO: -7.89674 LUMO: 0.31021 factor:1 | 1 (-0.28074) | 1 | 1 |
| G: -6322.69006 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.19353 HOMO: -7.26544 LUMO: 0.22858 factor:1 | 1 (-0.13777) | 1 | 1 |
| G: -6322.69006 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.33541 HOMO: -7.12666 LUMO: -0.02449 factor:1 | 1 (-0.27965) | 1 | 1 |
| G: -6322.69006 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.20477 HOMO: -7.68722 LUMO: 0.71838 factor:1 | 1 (-0.14901) | 1 | 1 |
| G: -6322.69006 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12586.96528 HOMO: -6.86271 LUMO: -0.96056 factor:1 | -1 (0.09048) | -1 | -1 |
| G: -6322.69006 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.44295 HOMO: -7.07496 LUMO: -1.11839 factor:1 | 1 (-0.38719) | 1 | 1 |
| G: -6322.69006 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.64031 HOMO: -7.06952 LUMO: -2.08439 factor:1 | 1 (-0.58455) | 1 | 1 |
| G: -6322.69006 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.83196 HOMO: -6.60965 LUMO: -2.11977 factor:1 | 1 (-0.77620) | -1 | -1 |
| G: -6322.69006 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.81838 HOMO: -6.87360 LUMO: -1.85854 factor:1 | 1 (-0.76263) | -1 | -1 |
| G: -6322.69006 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.61079 HOMO: -7.67089 LUMO: -0.24762 factor:1 | 1 (-0.55503) | 1 | 1 |
| G: -6322.69006 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.80676 HOMO: -6.45726 LUMO: -1.86398 factor:1 | 1 (-0.75101) | -1 | -1 |
| G: -6322.69006 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.81397 HOMO: -6.91713 LUMO: 0.33198 factor:1 | 1 (-0.75822) | -1 | -1 |
| G: -6322.69006 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.91980 HOMO: -6.83278 LUMO: 0.26667 factor:1 | 1 (-0.86404) | -1 | -1 |
| G: -6322.69006 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.69683 HOMO: -6.89264 LUMO: -1.00682 factor:1 | 1 (-0.64107) | -1 | -1 |
| G: -6322.69006 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.61838 HOMO: -6.57427 LUMO: 0.22041 factor:1 | 1 (-0.56262) | -1 | -1 |
| G: -6322.69006 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.60265 HOMO: -7.52123 LUMO: -0.01905 factor:1 | 1 (-0.54689) | 1 | 1 |
| G: -6322.69006 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.46610 HOMO: -7.37429 LUMO: -0.08980 factor:1 | 1 (-0.41035) | 1 | 1 |
| G: -6322.69006 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.39862 HOMO: -7.28449 LUMO: -0.26395 factor:1 | 1 (-0.34286) | 1 | 1 |
| G: -6322.69006 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.45351 HOMO: -6.79740 LUMO: -0.60954 factor:1 | 1 (-0.39775) | -1 | -1 |
| G: -6322.69006 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.47688 HOMO: -7.12666 LUMO: -0.60681 factor:1 | 1 (-0.42112) | 1 | 1 |
| G: -6322.69006 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.38599 HOMO: -6.96611 LUMO: -0.30477 factor:1 | 1 (-0.33024) | -1 | -1 |
| G: -6322.69006 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.67033 HOMO: -7.08040 LUMO: -0.31293 factor:1 | 1 (-0.61457) | 1 | 1 |
| G: -6322.69006 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.66442 HOMO: -6.78924 LUMO: -0.73743 factor:1 | 1 (-0.60866) | -1 | -1 |
| G: -6322.69006 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.67767 HOMO: -7.57293 LUMO: -1.11295 factor:1 | 1 (-0.62192) | 1 | 1 |
| G: -6322.69006 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.59743 HOMO: -7.15932 LUMO: -0.23130 factor:1 | 1 (-0.54167) | 1 | 1 |
| G: -6322.69006 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.35639 HOMO: -7.48585 LUMO: -0.10068 factor:1 | 1 (-0.30063) | 1 | 1 |
| G: -6322.69006 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.45541 HOMO: -7.17020 LUMO: -0.26123 factor:1 | 1 (-0.39965) | 1 | 1 |
| G: -6322.69006 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.39625 HOMO: -7.43143 LUMO: -0.16055 factor:1 | 1 (-0.34050) | 1 | 1 |
| G: -6322.69006 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.25522 HOMO: -7.14843 LUMO: -0.10612 factor:1 | 1 (-0.19946) | 1 | 1 |
| G: -6322.69006 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.51952 HOMO: -6.95523 LUMO: -0.22585 factor:1 | 1 (-0.46376) | -1 | -1 |
| G: -6322.69006 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.83389 HOMO: -7.06680 LUMO: -0.51974 factor:1 | 1 (-0.77814) | 1 | 1 |
| G: -6322.69006 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.53892 HOMO: -6.80829 LUMO: -0.64763 factor:1 | 1 (-0.48317) | -1 | -1 |
| G: -6322.69006 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.59070 HOMO: -7.13210 LUMO: -0.48164 factor:1 | 1 (-0.53495) | 1 | 1 |
| G: -6322.69006 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.66608 HOMO: -7.16204 LUMO: -0.45715 factor:1 | 1 (-0.61032) | 1 | 1 |
| G: -6322.69006 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.74687 HOMO: -7.15115 LUMO: -0.43266 factor:1 | 1 (-0.69111) | 1 | 1 |
| G: -6322.69006 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.70246 HOMO: -7.15932 LUMO: -2.52794 factor:1 | 1 (-0.64671) | -1 | -1 |
| G: -6322.69006 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.38719 HOMO: -7.21102 LUMO: -2.65311 factor:1 | 1 (-0.33143) | -1 | -1 |
| G: -6322.69006 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.54673 HOMO: -6.57427 LUMO: -2.78645 factor:1 | 1 (-0.49098) | -1 | -1 |
| G: -6322.69006 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.38009 HOMO: -6.40828 LUMO: -3.23815 factor:1 | 1 (-0.32433) | -1 | -1 |
| G: -6322.69006 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.74995 HOMO: -7.71987 LUMO: -0.20953 factor:1 | 1 (-0.69419) | 1 | 1 |
| G: -6322.69006 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.69033 HOMO: -7.47769 LUMO: -0.43810 factor:1 | 1 (-0.63457) | 1 | 1 |
| G: -6322.69006 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.63841 HOMO: -6.68040 LUMO: -2.22589 factor:1 | 1 (-0.58265) | -1 | -1 |
| G: -6322.69006 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.36512 HOMO: -6.92802 LUMO: -1.99187 factor:1 | 1 (-0.30937) | -1 | -1 |
| G: -6322.69006 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.43827 HOMO: -7.73620 LUMO: 0.01633 factor:1 | 1 (-0.38251) | 1 | 1 |
| G: -6322.69006 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.30986 HOMO: -7.28721 LUMO: -0.18504 factor:1 | 1 (-0.25410) | 1 | 1 |
| G: -6322.69006 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.19628 HOMO: -7.49674 LUMO: -0.19864 factor:1 | 1 (-0.14052) | 1 | 1 |
| G: -6322.69006 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12586.98457 HOMO: -7.10489 LUMO: -2.56331 factor:1 | -1 (0.07118) | -1 | -1 |
| G: -6322.69006 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.52787 HOMO: -7.36612 LUMO: 0.16055 factor:1 | 1 (-0.47212) | 1 | 1 |
| G: -6322.69006 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.40319 HOMO: -7.67633 LUMO: 0.33198 factor:1 | 1 (-0.34743) | 1 | 1 |
| G: -6322.86767 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12588.02195 HOMO: -7.07768 LUMO: -0.27483 factor:1 | 1 (-0.78859) | 1 | 1 |
| G: -6322.86767 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12588.08797 HOMO: -7.32531 LUMO: 0.05442 factor:1 | 1 (-0.85460) | 1 | 1 |
| G: -6322.86767 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12588.15719 HOMO: -6.79740 LUMO: -1.21635 factor:1 | 1 (-0.92383) | -1 | -1 |
| G: -6322.86767 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.78918 HOMO: -7.14027 LUMO: 0.12517 factor:1 | 1 (-0.55582) | 1 | -1 |
| G: -6322.86767 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.85993 HOMO: -7.17292 LUMO: 0.16871 factor:1 | 1 (-0.62657) | 1 | -1 |
| G: -6322.86767 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.69441 HOMO: -7.08312 LUMO: -1.38778 factor:1 | 1 (-0.46104) | 1 | 1 |
| G: -6322.86767 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12588.07695 HOMO: -6.75387 LUMO: -1.88031 factor:1 | 1 (-0.84358) | -1 | -1 |
| G: -6322.86767 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12588.08105 HOMO: -7.07768 LUMO: -1.25717 factor:1 | 1 (-0.84769) | 1 | 1 |
| G: -6322.86767 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.76791 HOMO: -6.46543 LUMO: -1.14016 factor:1 | 1 (-0.53454) | -1 | -1 |
| G: -6322.86767 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.67101 HOMO: -7.37973 LUMO: -0.45987 factor:1 | 1 (-0.43764) | 1 | 1 |
| G: -6322.86767 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.88989 HOMO: -7.46408 LUMO: 0.03265 factor:1 | 1 (-0.65653) | 1 | 1 |
| G: -6322.86767 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.50722 HOMO: -7.96477 LUMO: -0.19864 factor:1 | 1 (-0.27386) | 1 | 1 |
| G: -6322.86767 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.67724 HOMO: -6.93890 LUMO: -1.11839 factor:1 | 1 (-0.44387) | -1 | -1 |
| G: -6322.86767 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.71941 HOMO: -7.06408 LUMO: -1.08846 factor:1 | 1 (-0.48605) | 1 | 1 |
| G: -6322.86767 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.84644 HOMO: -7.14027 LUMO: -0.33470 factor:1 | 1 (-0.61307) | 1 | 1 |
| G: -6322.86767 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.95455 HOMO: -7.38245 LUMO: 0.10885 factor:1 | 1 (-0.72118) | 1 | 1 |
| G: -6322.86767 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.61090 HOMO: -7.59470 LUMO: -1.21363 factor:1 | 1 (-0.37753) | 1 | 1 |
| G: -6322.86767 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.66499 HOMO: -7.23279 LUMO: -1.23812 factor:1 | 1 (-0.43163) | 1 | 1 |
| G: -6322.86767 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.86538 HOMO: -6.90897 LUMO: 0.23402 factor:1 | 1 (-0.63201) | -1 | -1 |
| G: -6322.86767 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.86747 HOMO: -7.36340 LUMO: -0.17143 factor:1 | 1 (-0.63411) | 1 | 1 |
| G: -6322.86767 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.76527 HOMO: -6.61781 LUMO: -0.01361 factor:1 | 1 (-0.53190) | -1 | -1 |
| G: -6322.86767 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12588.05330 HOMO: -6.80013 LUMO: 0.38368 factor:1 | 1 (-0.81993) | -1 | -1 |
| G: -6322.86767 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.67560 HOMO: -6.72121 LUMO: -0.95512 factor:1 | 1 (-0.44224) | -1 | -1 |
| G: -6322.86767 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.47318 HOMO: -6.24773 LUMO: -0.69933 factor:1 | 1 (-0.23981) | -1 | -1 |
| G: -6322.86767 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.61928 HOMO: -6.56883 LUMO: 0.14694 factor:1 | 1 (-0.38591) | -1 | -1 |
| G: -6322.86767 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.67305 HOMO: -6.51441 LUMO: -1.27621 factor:1 | 1 (-0.43968) | -1 | -1 |
| G: -6322.86767 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.66535 HOMO: -6.91986 LUMO: -1.16737 factor:1 | 1 (-0.43198) | -1 | -1 |
| G: -6322.86767 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.56717 HOMO: -6.17971 LUMO: -0.65307 factor:1 | 1 (-0.33380) | -1 | -1 |
| G: -6322.86767 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.44978 HOMO: -7.22462 LUMO: 0.04354 factor:1 | 1 (-0.21641) | 1 | 1 |
| G: -6322.86767 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.25987 HOMO: -7.16204 LUMO: -0.23674 factor:1 | 1 (-0.02650) | 1 | 1 |
| G: -6322.86767 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.42795 HOMO: -6.81645 LUMO: -0.19320 factor:1 | 1 (-0.19459) | -1 | -1 |
| G: -6322.86767 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12588.04734 HOMO: -6.69400 LUMO: 0.04082 factor:1 | 1 (-0.81397) | -1 | -1 |
| G: -6322.86767 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.75074 HOMO: -6.63141 LUMO: -0.22858 factor:1 | 1 (-0.51737) | -1 | -1 |
| G: -6322.86767 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.73574 HOMO: -6.92258 LUMO: -1.11295 factor:1 | 1 (-0.50238) | -1 | -1 |
| G: -6322.86767 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.98834 HOMO: -6.60148 LUMO: -1.13744 factor:1 | 1 (-0.75498) | -1 | -1 |
| G: -6322.86767 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.66102 HOMO: -6.78108 LUMO: -0.82450 factor:1 | 1 (-0.42765) | -1 | -1 |
| G: -6322.86767 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.83457 HOMO: -7.05591 LUMO: -0.97145 factor:1 | 1 (-0.60121) | -1 | -1 |
| G: -6322.86767 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.92976 HOMO: -6.65318 LUMO: -1.26261 factor:1 | 1 (-0.69639) | -1 | -1 |
| G: -6322.86767 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.78118 HOMO: -6.98244 LUMO: -0.98233 factor:1 | 1 (-0.54782) | -1 | -1 |
| G: -6322.86767 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.50357 HOMO: -7.11850 LUMO: -0.99594 factor:1 | 1 (-0.27021) | 1 | 1 |
| G: -6322.86767 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.41321 HOMO: -6.64230 LUMO: -0.93879 factor:1 | 1 (-0.17984) | -1 | -1 |
| G: -6322.86767 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.73063 HOMO: -6.62053 LUMO: -1.22451 factor:1 | 1 (-0.49726) | -1 | -1 |
| G: -6322.86767 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.59851 HOMO: -7.02598 LUMO: -0.85172 factor:1 | 1 (-0.36515) | -1 | -1 |
| G: -6322.86767 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.74622 HOMO: -7.06680 LUMO: -0.89253 factor:1 | 1 (-0.51285) | 1 | 1 |
| G: -6322.86767 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.70526 HOMO: -7.17292 LUMO: 0.00272 factor:1 | 1 (-0.47190) | 1 | 1 |
| G: -6322.86767 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.59541 HOMO: -7.03142 LUMO: -0.35103 factor:1 | 1 (-0.36205) | -1 | -1 |
| G: -6322.86767 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.94924 HOMO: -6.96884 LUMO: -0.09796 factor:1 | 1 (-0.71588) | -1 | -1 |
| G: -6322.86767 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.73642 HOMO: -6.56339 LUMO: -0.99322 factor:1 | 1 (-0.50306) | -1 | -1 |
| G: -6322.86767 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.66611 HOMO: -7.08857 LUMO: -0.17687 factor:1 | 1 (-0.43274) | 1 | 1 |
| G: -6322.86767 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.60837 HOMO: -7.05863 LUMO: -0.22041 factor:1 | 1 (-0.37500) | -1 | -1 |
| G: -6322.86767 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.43944 HOMO: -7.15115 LUMO: -0.17960 factor:1 | 1 (-0.20607) | 1 | 1 |
| G: -6322.86767 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.51274 HOMO: -6.67495 LUMO: -0.96600 factor:1 | 1 (-0.27938) | -1 | -1 |
| G: -6322.86767 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.68897 HOMO: -6.74026 LUMO: -1.79867 factor:1 | 1 (-0.45560) | -1 | -1 |
| G: -6322.86767 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.72317 HOMO: -6.73482 LUMO: -1.78235 factor:1 | 1 (-0.48980) | -1 | -1 |
| G: -6322.86767 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.83591 HOMO: -6.09807 LUMO: 0.16871 factor:1 | 1 (-0.60254) | -1 | -1 |
| G: -6322.86767 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.56306 HOMO: -6.72393 LUMO: 0.27211 factor:1 | 1 (-0.32969) | -1 | -1 |
| G: -6322.86767 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.43650 HOMO: -6.40556 LUMO: -0.04354 factor:1 | 1 (-0.20313) | -1 | -1 |
| G: -6322.86767 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.40510 HOMO: -6.56883 LUMO: 0.22041 factor:1 | 1 (-0.17173) | -1 | -1 |
| G: -6322.86767 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.20942 HOMO: -7.22462 LUMO: 0.15783 factor:1 | -1 (0.02395) | 1 | 1 |
| G: -6322.86767 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.86867 HOMO: -6.83550 LUMO: 0.19320 factor:1 | 1 (-0.63530) | -1 | -1 |
| G: -6322.86767 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.75710 HOMO: -7.26816 LUMO: -0.07619 factor:1 | 1 (-0.52374) | 1 | -1 |
| G: -6322.86767 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.63536 HOMO: -7.13483 LUMO: 0.33198 factor:1 | 1 (-0.40199) | 1 | 1 |
| G: -6322.86767 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.64581 HOMO: -6.58243 LUMO: -0.26395 factor:1 | 1 (-0.41244) | -1 | -1 |
| G: -6322.86767 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.80742 HOMO: -7.38517 LUMO: 0.17143 factor:1 | 1 (-0.57405) | 1 | 1 |
| G: -6322.86767 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.69180 HOMO: -6.80013 LUMO: 0.25851 factor:1 | 1 (-0.45843) | -1 | -1 |
| G: -6322.86767 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.89811 HOMO: -6.96611 LUMO: 0.11429 factor:1 | 1 (-0.66475) | -1 | -1 |
| G: -6322.86767 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.84276 HOMO: -6.51713 LUMO: -1.14560 factor:1 | 1 (-0.60940) | -1 | -1 |
| G: -6322.86767 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.61158 HOMO: -7.15387 LUMO: -0.35647 factor:1 | 1 (-0.37821) | 1 | 1 |
| G: -6322.86767 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.52845 HOMO: -5.26540 LUMO: 1.26805 factor:1 | 1 (-0.29508) | -1 | -1 |
| G: -6322.86767 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.53468 HOMO: -6.76475 LUMO: -0.16327 factor:1 | 1 (-0.30131) | -1 | -1 |
| G: -6322.86767 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.42469 HOMO: -6.55250 LUMO: -0.71838 factor:1 | 1 (-0.19132) | -1 | -1 |
| G: -6322.86767 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.94908 HOMO: -6.76203 LUMO: -1.08301 factor:1 | 1 (-0.71571) | -1 | -1 |
| G: -6322.86767 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.71463 HOMO: -7.14027 LUMO: -0.01633 factor:1 | 1 (-0.48126) | 1 | 1 |
| G: -6322.86767 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.59819 HOMO: -6.94979 LUMO: -0.93879 factor:1 | 1 (-0.36482) | -1 | -1 |
| G: -6322.86767 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.76663 HOMO: -6.74842 LUMO: 0.31293 factor:1 | 1 (-0.53326) | -1 | -1 |
| G: -6322.86767 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.47653 HOMO: -6.43821 LUMO: 0.05987 factor:1 | 1 (-0.24316) | -1 | -1 |
| G: -6322.86767 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.49057 HOMO: -6.60420 LUMO: 0.22585 factor:1 | 1 (-0.25720) | -1 | -1 |
| G: -6322.86767 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.34504 HOMO: -6.43821 LUMO: 0.05987 factor:1 | 1 (-0.11168) | -1 | -1 |
| G: -6322.86767 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.61500 HOMO: -6.34570 LUMO: 1.43948 factor:1 | 1 (-0.38164) | -1 | -1 |
| G: -6322.86767 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.33919 HOMO: -6.03004 LUMO: 1.21363 factor:1 | 1 (-0.10583) | -1 | -1 |
| G: -6322.86767 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.33650 HOMO: -6.68040 LUMO: -0.92247 factor:1 | 1 (-0.10313) | -1 | -1 |
| G: -6322.86767 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.19353 HOMO: -6.92530 LUMO: -0.31293 factor:1 | -1 (0.03984) | -1 | -1 |
| G: -6322.86767 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.33541 HOMO: -6.94979 LUMO: -0.19864 factor:1 | 1 (-0.10204) | -1 | -1 |
| G: -6322.86767 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.20477 HOMO: -6.80829 LUMO: -0.30477 factor:1 | -1 (0.02860) | -1 | -1 |
| G: -6322.86767 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12586.96528 HOMO: -7.22734 LUMO: -1.02859 factor:1 | -1 (0.26809) | 1 | 1 |
| G: -6322.86767 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.44295 HOMO: -6.93890 LUMO: -0.72382 factor:1 | 1 (-0.20958) | -1 | -1 |
| G: -6322.86767 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.64031 HOMO: -7.27088 LUMO: -0.78097 factor:1 | 1 (-0.40695) | 1 | 1 |
| G: -6322.86767 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.83196 HOMO: -7.29809 LUMO: -0.97145 factor:1 | 1 (-0.59860) | 1 | 1 |
| G: -6322.86767 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.81838 HOMO: -7.18925 LUMO: -0.94696 factor:1 | 1 (-0.58502) | 1 | 1 |
| G: -6322.86767 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.61079 HOMO: -7.33891 LUMO: -0.96873 factor:1 | 1 (-0.37742) | 1 | 1 |
| G: -6322.86767 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.80676 HOMO: -7.36068 LUMO: -0.28028 factor:1 | 1 (-0.57340) | 1 | 1 |
| G: -6322.86767 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.81397 HOMO: -7.10761 LUMO: -1.14832 factor:1 | 1 (-0.58061) | 1 | 1 |
| G: -6322.86767 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.91980 HOMO: -6.94707 LUMO: -0.65307 factor:1 | 1 (-0.68643) | -1 | -1 |
| G: -6322.86767 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.69683 HOMO: -6.91713 LUMO: -1.81228 factor:1 | 1 (-0.46346) | -1 | -1 |
| G: -6322.86767 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.61838 HOMO: -6.78652 LUMO: -2.01636 factor:1 | 1 (-0.38501) | -1 | -1 |
| G: -6322.86767 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.60265 HOMO: -6.52801 LUMO: -1.17553 factor:1 | 1 (-0.36929) | -1 | -1 |
| G: -6322.86767 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.46610 HOMO: -7.54844 LUMO: -1.18642 factor:1 | 1 (-0.23274) | 1 | -1 |
| G: -6322.86767 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.39862 HOMO: -7.52939 LUMO: -1.23812 factor:1 | 1 (-0.16525) | 1 | -1 |
| G: -6322.86767 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.45351 HOMO: -7.94572 LUMO: -0.81634 factor:1 | 1 (-0.22014) | 1 | 1 |
| G: -6322.86767 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.47688 HOMO: -7.55932 LUMO: -0.86260 factor:1 | 1 (-0.24351) | 1 | 1 |
| G: -6322.86767 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.38599 HOMO: -7.72259 LUMO: -1.39050 factor:1 | 1 (-0.15263) | 1 | -1 |
| G: -6322.86767 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.67033 HOMO: -7.11850 LUMO: -1.01498 factor:1 | 1 (-0.43696) | 1 | -1 |
| G: -6322.86767 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.66442 HOMO: -7.09673 LUMO: -1.00954 factor:1 | 1 (-0.43106) | 1 | -1 |
| G: -6322.86767 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.67767 HOMO: -6.06270 LUMO: 0.16327 factor:1 | 1 (-0.44431) | -1 | -1 |
| G: -6322.86767 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.59743 HOMO: -5.71167 LUMO: 0.70477 factor:1 | 1 (-0.36406) | -1 | -1 |
| G: -6322.86767 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.35639 HOMO: -5.38241 LUMO: 0.86260 factor:1 | 1 (-0.12302) | -1 | -1 |
| G: -6322.86767 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.45541 HOMO: -5.67357 LUMO: 1.27621 factor:1 | 1 (-0.22204) | -1 | -1 |
| G: -6322.86767 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.39625 HOMO: -7.56204 LUMO: -0.68573 factor:1 | 1 (-0.16289) | 1 | 1 |
| G: -6322.86767 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.25522 HOMO: -5.57833 LUMO: 1.13199 factor:1 | 1 (-0.02185) | -1 | -1 |
| G: -6322.86767 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.51952 HOMO: -7.58653 LUMO: -0.66124 factor:1 | 1 (-0.28615) | 1 | 1 |
| G: -6322.86767 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.83389 HOMO: -7.91851 LUMO: -1.10206 factor:1 | 1 (-0.60053) | 1 | -1 |
| G: -6322.86767 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.53892 HOMO: -6.48992 LUMO: -1.00138 factor:1 | 1 (-0.30556) | -1 | -1 |
| G: -6322.86767 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.59070 HOMO: -7.09673 LUMO: -0.45171 factor:1 | 1 (-0.35734) | 1 | 1 |
| G: -6322.86767 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.66608 HOMO: -6.63686 LUMO: 0.09252 factor:1 | 1 (-0.43272) | -1 | -1 |
| G: -6322.86767 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.74687 HOMO: -6.84366 LUMO: -0.14422 factor:1 | 1 (-0.51351) | -1 | -1 |
| G: -6322.86767 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.70246 HOMO: -6.93074 LUMO: 0.04354 factor:1 | 1 (-0.46910) | -1 | -1 |
| G: -6322.86767 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.38719 HOMO: -6.90353 LUMO: -0.19864 factor:1 | 1 (-0.15383) | -1 | -1 |
| G: -6322.86767 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.54673 HOMO: -6.59876 LUMO: -0.10068 factor:1 | 1 (-0.31337) | -1 | -1 |
| G: -6322.86767 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.38009 HOMO: -6.74570 LUMO: -0.44627 factor:1 | 1 (-0.14672) | -1 | -1 |
| G: -6322.86767 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.74995 HOMO: -6.60148 LUMO: -0.61770 factor:1 | 1 (-0.51658) | -1 | -1 |
| G: -6322.86767 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.69033 HOMO: -6.55794 LUMO: -1.06941 factor:1 | 1 (-0.45696) | -1 | -1 |
| G: -6322.86767 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.63841 HOMO: -7.12666 LUMO: -0.11973 factor:1 | 1 (-0.40504) | 1 | 1 |
| G: -6322.86767 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.36512 HOMO: -7.21646 LUMO: -0.50069 factor:1 | 1 (-0.13176) | 1 | 1 |
| G: -6322.86767 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.43827 HOMO: -7.27632 LUMO: -1.00682 factor:1 | 1 (-0.20490) | 1 | -1 |
| G: -6322.86767 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.30986 HOMO: -6.74298 LUMO: 0.04354 factor:1 | 1 (-0.07649) | -1 | -1 |
| G: -6322.86767 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.19628 HOMO: -6.37291 LUMO: 0.14150 factor:1 | -1 (0.03709) | -1 | -1 |
| G: -6322.86767 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12586.98457 HOMO: -5.61371 LUMO: 1.28438 factor:1 | -1 (0.24879) | -1 | -1 |
| G: -6322.86767 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.52787 HOMO: -5.52119 LUMO: 0.99866 factor:1 | 1 (-0.29451) | -1 | -1 |
| G: -6322.86767 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.40319 HOMO: -6.51985 LUMO: -0.10885 factor:1 | 1 (-0.16983) | -1 | -1 |
| G: -6322.76761 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12588.02195 HOMO: -5.61371 LUMO: 0.77280 factor:1 | 1 (-0.88864) | -1 | -1 |
| G: -6322.76761 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12588.08797 HOMO: -5.58922 LUMO: 0.24490 factor:1 | 1 (-0.95466) | -1 | -1 |
| G: -6322.76761 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12588.15719 HOMO: -6.32665 LUMO: -0.57144 factor:1 | 1 (-1.02388) | -1 | -1 |
| G: -6322.76761 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.78918 HOMO: -6.29127 LUMO: -0.93607 factor:1 | 1 (-0.65588) | -1 | -1 |
| G: -6322.76761 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.85993 HOMO: -5.49670 LUMO: 0.27211 factor:1 | 1 (-0.72663) | -1 | -1 |
| G: -6322.76761 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.69441 HOMO: -5.68990 LUMO: 0.24218 factor:1 | 1 (-0.56110) | -1 | -1 |
| G: -6322.76761 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12588.07695 HOMO: -5.68174 LUMO: 0.69933 factor:1 | 1 (-0.94364) | -1 | -1 |
| G: -6322.76761 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12588.08105 HOMO: -5.28173 LUMO: 1.00954 factor:1 | 1 (-0.94775) | -1 | -1 |
| G: -6322.76761 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.76791 HOMO: -5.94025 LUMO: 0.73471 factor:1 | 1 (-0.63460) | -1 | -1 |
| G: -6322.76761 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.67101 HOMO: -5.65725 LUMO: 1.28710 factor:1 | 1 (-0.53770) | -1 | -1 |
| G: -6322.76761 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.88989 HOMO: -5.41507 LUMO: 0.87076 factor:1 | 1 (-0.75659) | -1 | -1 |
| G: -6322.76761 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.50722 HOMO: -5.96474 LUMO: 0.29660 factor:1 | 1 (-0.37391) | -1 | -1 |
| G: -6322.76761 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.67724 HOMO: -7.00421 LUMO: 0.08708 factor:1 | 1 (-0.54393) | -1 | -1 |
| G: -6322.76761 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.71941 HOMO: -5.40418 LUMO: 0.90070 factor:1 | 1 (-0.58611) | -1 | -1 |
| G: -6322.76761 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.84644 HOMO: -7.00421 LUMO: -0.30477 factor:1 | 1 (-0.71313) | -1 | -1 |
| G: -6322.76761 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.95455 HOMO: -5.85861 LUMO: 0.74015 factor:1 | 1 (-0.82124) | -1 | -1 |
| G: -6322.76761 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.61090 HOMO: -5.71439 LUMO: 0.26395 factor:1 | 1 (-0.47759) | -1 | -1 |
| G: -6322.76761 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.66499 HOMO: -7.13755 LUMO: -0.78369 factor:1 | 1 (-0.53168) | 1 | -1 |
| G: -6322.76761 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.86538 HOMO: -7.31442 LUMO: -0.98233 factor:1 | 1 (-0.73207) | 1 | -1 |
| G: -6322.76761 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.86747 HOMO: -7.25728 LUMO: -1.00410 factor:1 | 1 (-0.73416) | 1 | -1 |
| G: -6322.76761 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.76527 HOMO: -7.48585 LUMO: -0.83811 factor:1 | 1 (-0.63196) | 1 | -1 |
| G: -6322.76761 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12588.05330 HOMO: -7.24911 LUMO: -0.77280 factor:1 | 1 (-0.91999) | 1 | -1 |
| G: -6322.76761 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.67560 HOMO: -7.55116 LUMO: -1.19730 factor:1 | 1 (-0.54230) | 1 | -1 |
| G: -6322.76761 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.47318 HOMO: -5.76881 LUMO: 0.28028 factor:1 | 1 (-0.33987) | -1 | -1 |
| G: -6322.76761 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.61928 HOMO: -5.77153 LUMO: -0.26939 factor:1 | 1 (-0.48597) | -1 | -1 |
| G: -6322.76761 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.67305 HOMO: -5.82868 LUMO: 0.36735 factor:1 | 1 (-0.53974) | -1 | -1 |
| G: -6322.76761 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.66535 HOMO: -5.83140 LUMO: -0.17960 factor:1 | 1 (-0.53204) | -1 | -1 |
| G: -6322.76761 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.56717 HOMO: -6.28855 LUMO: 0.01088 factor:1 | 1 (-0.43386) | -1 | -1 |
| G: -6322.76761 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.44978 HOMO: -6.31576 LUMO: 0.25307 factor:1 | 1 (-0.31647) | -1 | -1 |
| G: -6322.76761 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.25987 HOMO: -7.06408 LUMO: -2.76196 factor:1 | 1 (-0.12656) | -1 | -1 |
| G: -6322.76761 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.42795 HOMO: -5.95657 LUMO: 0.37552 factor:1 | 1 (-0.29464) | -1 | -1 |
| G: -6322.76761 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12588.04734 HOMO: -6.61781 LUMO: 0.02721 factor:1 | 1 (-0.91403) | -1 | -1 |
| G: -6322.76761 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.75074 HOMO: -6.26678 LUMO: -0.66668 factor:1 | 1 (-0.61743) | -1 | -1 |
| G: -6322.76761 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.73574 HOMO: -6.00011 LUMO: -0.13334 factor:1 | 1 (-0.60243) | -1 | -1 |
| G: -6322.76761 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.98834 HOMO: -5.60555 LUMO: 0.67484 factor:1 | 1 (-0.85504) | -1 | -1 |
| G: -6322.76761 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.66102 HOMO: -5.79875 LUMO: 0.99049 factor:1 | 1 (-0.52771) | -1 | -1 |
| G: -6322.76761 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.83457 HOMO: -5.97834 LUMO: 0.48436 factor:1 | 1 (-0.70126) | -1 | -1 |
| G: -6322.76761 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.92976 HOMO: -5.82868 LUMO: 0.91974 factor:1 | 1 (-0.79645) | -1 | -1 |
| G: -6322.76761 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.78118 HOMO: -5.86677 LUMO: 0.99594 factor:1 | 1 (-0.64788) | -1 | -1 |
| G: -6322.76761 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.50357 HOMO: -5.70079 LUMO: 0.48980 factor:1 | 1 (-0.37027) | -1 | -1 |
| G: -6322.76761 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.41321 HOMO: -7.39605 LUMO: -1.02315 factor:1 | 1 (-0.27990) | 1 | -1 |
| G: -6322.76761 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.73063 HOMO: -7.22734 LUMO: -1.12927 factor:1 | 1 (-0.59732) | 1 | -1 |
| G: -6322.76761 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.59851 HOMO: -7.58926 LUMO: -0.65035 factor:1 | 1 (-0.46521) | 1 | 1 |
| G: -6322.76761 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.74622 HOMO: -7.43959 LUMO: -0.75648 factor:1 | 1 (-0.61291) | 1 | 1 |
| G: -6322.76761 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.70526 HOMO: -7.55388 LUMO: -1.15104 factor:1 | 1 (-0.57196) | 1 | -1 |
| G: -6322.76761 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.59541 HOMO: -6.74570 LUMO: -2.85447 factor:1 | 1 (-0.46210) | -1 | -1 |
| G: -6322.76761 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.94924 HOMO: -7.35524 LUMO: -1.25444 factor:1 | 1 (-0.81593) | 1 | 1 |
| G: -6322.76761 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.73642 HOMO: -6.81645 LUMO: -1.20819 factor:1 | 1 (-0.60311) | -1 | -1 |
| G: -6322.76761 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.66611 HOMO: -6.99605 LUMO: -1.62996 factor:1 | 1 (-0.53280) | -1 | -1 |
| G: -6322.76761 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.60837 HOMO: -6.88992 LUMO: -0.47620 factor:1 | 1 (-0.47506) | -1 | -1 |
| G: -6322.76761 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.43944 HOMO: -7.22190 LUMO: -0.01905 factor:1 | 1 (-0.30613) | 1 | 1 |
| G: -6322.76761 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.51274 HOMO: -6.77836 LUMO: -0.82995 factor:1 | 1 (-0.37944) | -1 | -1 |
| G: -6322.76761 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.68897 HOMO: -6.48447 LUMO: -0.95512 factor:1 | 1 (-0.55566) | -1 | -1 |
| G: -6322.76761 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.72317 HOMO: -7.81239 LUMO: 1.22179 factor:1 | 1 (-0.58986) | 1 | 1 |
| G: -6322.76761 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.83591 HOMO: -7.36612 LUMO: 0.19320 factor:1 | 1 (-0.70260) | 1 | 1 |
| G: -6322.76761 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.56306 HOMO: -7.24095 LUMO: 0.33470 factor:1 | 1 (-0.42975) | 1 | 1 |
| G: -6322.76761 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.43650 HOMO: -7.15932 LUMO: -2.24222 factor:1 | 1 (-0.30319) | -1 | -1 |
| G: -6322.76761 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.40510 HOMO: -6.88992 LUMO: -2.69937 factor:1 | 1 (-0.27179) | -1 | -1 |
| G: -6322.76761 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.20942 HOMO: -6.97428 LUMO: -0.98233 factor:1 | 1 (-0.07611) | -1 | -1 |
| G: -6322.76761 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.86867 HOMO: -7.17564 LUMO: -0.93879 factor:1 | 1 (-0.73536) | 1 | 1 |
| G: -6322.76761 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.75710 HOMO: -6.81645 LUMO: -1.14288 factor:1 | 1 (-0.62379) | -1 | -1 |
| G: -6322.76761 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.63536 HOMO: -6.83006 LUMO: -0.63403 factor:1 | 1 (-0.50205) | -1 | -1 |
| G: -6322.76761 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.64581 HOMO: -7.17292 LUMO: -1.07213 factor:1 | 1 (-0.51250) | 1 | 1 |
| G: -6322.76761 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.80742 HOMO: -7.53755 LUMO: 0.15510 factor:1 | 1 (-0.67411) | 1 | 1 |
| G: -6322.76761 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.69180 HOMO: -6.50080 LUMO: -0.51702 factor:1 | 1 (-0.55849) | -1 | -1 |
| G: -6322.76761 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.89811 HOMO: -6.72665 LUMO: -0.80001 factor:1 | 1 (-0.76480) | -1 | -1 |
| G: -6322.76761 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.84276 HOMO: -6.72665 LUMO: 1.68711 factor:1 | 1 (-0.70946) | -1 | -1 |
| G: -6322.76761 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.61158 HOMO: -7.11850 LUMO: -0.75103 factor:1 | 1 (-0.47827) | 1 | 1 |
| G: -6322.76761 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.52845 HOMO: -6.87087 LUMO: -0.85988 factor:1 | 1 (-0.39514) | -1 | -1 |
| G: -6322.76761 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.53468 HOMO: -7.08857 LUMO: -0.89798 factor:1 | 1 (-0.40137) | 1 | 1 |
| G: -6322.76761 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.42469 HOMO: -6.71305 LUMO: -0.85444 factor:1 | 1 (-0.29138) | -1 | -1 |
| G: -6322.76761 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.94908 HOMO: -6.59332 LUMO: -0.60137 factor:1 | 1 (-0.81577) | -1 | -1 |
| G: -6322.76761 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.71463 HOMO: -7.28993 LUMO: 0.03265 factor:1 | 1 (-0.58132) | 1 | 1 |
| G: -6322.76761 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.59819 HOMO: -7.32258 LUMO: 0.13878 factor:1 | 1 (-0.46488) | 1 | 1 |
| G: -6322.76761 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.76663 HOMO: -7.28993 LUMO: 0.11429 factor:1 | 1 (-0.63332) | 1 | 1 |
| G: -6322.76761 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.47653 HOMO: -6.86271 LUMO: -1.03947 factor:1 | 1 (-0.34322) | -1 | -1 |
| G: -6322.76761 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.49057 HOMO: -6.55794 LUMO: -0.84900 factor:1 | 1 (-0.35726) | -1 | -1 |
| G: -6322.76761 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.34504 HOMO: -7.03686 LUMO: 0.11429 factor:1 | 1 (-0.21173) | -1 | -1 |
| G: -6322.76761 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.61500 HOMO: -7.06952 LUMO: -0.96056 factor:1 | 1 (-0.48170) | 1 | 1 |
| G: -6322.76761 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.33919 HOMO: -6.90897 LUMO: -0.99866 factor:1 | 1 (-0.20588) | -1 | -1 |
| G: -6322.76761 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.33650 HOMO: -7.00693 LUMO: -0.83539 factor:1 | 1 (-0.20319) | -1 | -1 |
| G: -6322.76761 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.19353 HOMO: -6.74298 LUMO: -0.85172 factor:1 | 1 (-0.06022) | -1 | -1 |
| G: -6322.76761 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.33541 HOMO: -6.83822 LUMO: -1.07213 factor:1 | 1 (-0.20210) | -1 | -1 |
| G: -6322.76761 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.20477 HOMO: -7.21918 LUMO: -1.55377 factor:1 | 1 (-0.07146) | 1 | 1 |
| G: -6322.76761 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12586.96528 HOMO: -6.84094 LUMO: -1.09934 factor:1 | -1 (0.16803) | -1 | -1 |
| G: -6322.76761 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.44295 HOMO: -7.09129 LUMO: -0.85988 factor:1 | 1 (-0.30964) | 1 | 1 |
| G: -6322.76761 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.64031 HOMO: -6.57971 LUMO: -2.27215 factor:1 | 1 (-0.50700) | -1 | -1 |
| G: -6322.76761 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.83196 HOMO: -6.81373 LUMO: -1.86942 factor:1 | 1 (-0.69865) | -1 | -1 |
| G: -6322.76761 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.81838 HOMO: -6.59060 LUMO: -2.30480 factor:1 | 1 (-0.68507) | -1 | -1 |
| G: -6322.76761 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.61079 HOMO: -6.72938 LUMO: -1.23540 factor:1 | 1 (-0.47748) | -1 | -1 |
| G: -6322.76761 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.80676 HOMO: -6.94707 LUMO: -2.62318 factor:1 | 1 (-0.67345) | -1 | -1 |
| G: -6322.76761 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.81397 HOMO: -7.28177 LUMO: -0.09796 factor:1 | 1 (-0.68067) | 1 | 1 |
| G: -6322.76761 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.91980 HOMO: -6.80013 LUMO: -0.79729 factor:1 | 1 (-0.78649) | -1 | -1 |
| G: -6322.76761 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.69683 HOMO: -7.26544 LUMO: 0.12789 factor:1 | 1 (-0.56352) | 1 | 1 |
| G: -6322.76761 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.61838 HOMO: -6.51713 LUMO: -0.49253 factor:1 | 1 (-0.48507) | -1 | -1 |
| G: -6322.76761 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.60265 HOMO: -6.68856 LUMO: -0.77280 factor:1 | 1 (-0.46934) | -1 | -1 |
| G: -6322.76761 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.46610 HOMO: -6.41100 LUMO: -0.70750 factor:1 | 1 (-0.33280) | -1 | -1 |
| G: -6322.76761 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.39862 HOMO: -7.56204 LUMO: 0.22041 factor:1 | 1 (-0.26531) | 1 | 1 |
| G: -6322.76761 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.45351 HOMO: -6.68312 LUMO: 1.30343 factor:1 | 1 (-0.32020) | -1 | -1 |
| G: -6322.76761 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.47688 HOMO: -7.24367 LUMO: 0.17415 factor:1 | 1 (-0.34357) | 1 | 1 |
| G: -6322.76761 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.38599 HOMO: -7.52395 LUMO: 1.16737 factor:1 | 1 (-0.25268) | 1 | 1 |
| G: -6322.76761 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.67033 HOMO: -6.89264 LUMO: 0.23130 factor:1 | 1 (-0.53702) | -1 | -1 |
| G: -6322.76761 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.66442 HOMO: -7.21102 LUMO: 0.19048 factor:1 | 1 (-0.53111) | 1 | 1 |
| G: -6322.76761 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.67767 HOMO: -7.08312 LUMO: 0.25034 factor:1 | 1 (-0.54436) | 1 | 1 |
| G: -6322.76761 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.59743 HOMO: -6.49536 LUMO: -0.65852 factor:1 | 1 (-0.46412) | -1 | -1 |
| G: -6322.76761 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.35639 HOMO: -6.85455 LUMO: 0.13606 factor:1 | 1 (-0.22308) | -1 | -1 |
| G: -6322.76761 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.45541 HOMO: -7.10217 LUMO: 0.35919 factor:1 | 1 (-0.32210) | 1 | 1 |
| G: -6322.76761 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.39625 HOMO: -7.77429 LUMO: 1.19186 factor:1 | 1 (-0.26294) | 1 | 1 |
| G: -6322.76761 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.25522 HOMO: -6.57427 LUMO: -0.50069 factor:1 | 1 (-0.12191) | -1 | -1 |
| G: -6322.76761 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.51952 HOMO: -7.36340 LUMO: 0.10068 factor:1 | 1 (-0.38621) | 1 | 1 |
| G: -6322.76761 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.83389 HOMO: -7.28177 LUMO: 0.15238 factor:1 | 1 (-0.70058) | 1 | 1 |
| G: -6322.76761 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.53892 HOMO: -6.86543 LUMO: -0.84355 factor:1 | 1 (-0.40561) | -1 | -1 |
| G: -6322.76761 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.59070 HOMO: -6.55794 LUMO: 1.39594 factor:1 | 1 (-0.45740) | -1 | -1 |
| G: -6322.76761 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.66608 HOMO: -6.26134 LUMO: 1.53744 factor:1 | 1 (-0.53277) | -1 | -1 |
| G: -6322.76761 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.74687 HOMO: -5.97562 LUMO: 1.42316 factor:1 | 1 (-0.61356) | -1 | -1 |
| G: -6322.76761 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.70246 HOMO: -6.65046 LUMO: 1.44492 factor:1 | 1 (-0.56915) | -1 | -1 |
| G: -6322.76761 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.38719 HOMO: -6.92258 LUMO: 0.17415 factor:1 | 1 (-0.25388) | -1 | -1 |
| G: -6322.76761 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.54673 HOMO: -7.40966 LUMO: 0.19592 factor:1 | 1 (-0.41342) | 1 | 1 |
| G: -6322.76761 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.38009 HOMO: -7.17564 LUMO: 0.16871 factor:1 | 1 (-0.24678) | 1 | 1 |
| G: -6322.76761 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.74995 HOMO: -7.46953 LUMO: 0.22313 factor:1 | 1 (-0.61664) | 1 | 1 |
| G: -6322.76761 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.69033 HOMO: -6.13345 LUMO: 1.85854 factor:1 | 1 (-0.55702) | -1 | -1 |
| G: -6322.76761 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.63841 HOMO: -6.99333 LUMO: -1.65717 factor:1 | 1 (-0.50510) | -1 | -1 |
| G: -6322.76761 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.36512 HOMO: -6.93074 LUMO: -1.79323 factor:1 | 1 (-0.23181) | -1 | -1 |
| G: -6322.76761 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.43827 HOMO: -6.87904 LUMO: -1.79323 factor:1 | 1 (-0.30496) | -1 | -1 |
| G: -6322.76761 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.30986 HOMO: -6.84094 LUMO: 0.66940 factor:1 | 1 (-0.17655) | -1 | -1 |
| G: -6322.76761 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.19628 HOMO: -7.13210 LUMO: -1.17553 factor:1 | 1 (-0.06297) | 1 | 1 |
| G: -6322.76761 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12586.98457 HOMO: -6.52801 LUMO: -2.23678 factor:1 | -1 (0.14874) | -1 | -1 |
| G: -6322.76761 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.52787 HOMO: -6.81917 LUMO: -1.86398 factor:1 | 1 (-0.39457) | -1 | -1 |
| G: -6322.76761 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.40319 HOMO: -7.30626 LUMO: -1.66806 factor:1 | 1 (-0.26988) | 1 | 1 |
| G: -6322.92103 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12588.02195 HOMO: -6.98516 LUMO: -1.40683 factor:1 | 1 (-0.73522) | -1 | -1 |
| G: -6322.92103 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12588.08797 HOMO: -6.95523 LUMO: -0.97145 factor:1 | 1 (-0.80124) | -1 | -1 |
| G: -6322.92103 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12588.15719 HOMO: -6.83278 LUMO: -2.68848 factor:1 | 1 (-0.87047) | -1 | -1 |
| G: -6322.92103 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.78918 HOMO: -7.25456 LUMO: -2.97420 factor:1 | 1 (-0.50246) | -1 | -1 |
| G: -6322.92103 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.85993 HOMO: -6.80557 LUMO: -2.65039 factor:1 | 1 (-0.57321) | -1 | -1 |
| G: -6322.92103 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.69441 HOMO: -7.10489 LUMO: 0.77008 factor:1 | 1 (-0.40768) | 1 | -1 |
| G: -6322.92103 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12588.07695 HOMO: -7.28993 LUMO: -1.06124 factor:1 | 1 (-0.79022) | 1 | 1 |
| G: -6322.92103 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12588.08105 HOMO: -7.11578 LUMO: -1.10206 factor:1 | 1 (-0.79433) | 1 | 1 |
| G: -6322.92103 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.76791 HOMO: -6.91713 LUMO: -1.36329 factor:1 | 1 (-0.48118) | -1 | -1 |
| G: -6322.92103 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.67101 HOMO: -7.07224 LUMO: 0.51974 factor:1 | 1 (-0.38428) | 1 | 1 |
| G: -6322.92103 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.88989 HOMO: -7.22734 LUMO: -0.93335 factor:1 | 1 (-0.60317) | 1 | 1 |
| G: -6322.92103 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.50722 HOMO: -7.19469 LUMO: -0.96600 factor:1 | 1 (-0.22049) | 1 | 1 |
| G: -6322.92103 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.67724 HOMO: -6.93890 LUMO: -0.66940 factor:1 | 1 (-0.39051) | -1 | -1 |
| G: -6322.92103 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.71941 HOMO: -7.09673 LUMO: -1.05852 factor:1 | 1 (-0.43269) | 1 | 1 |
| G: -6322.92103 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.84644 HOMO: -7.19197 LUMO: -2.26943 factor:1 | 1 (-0.55971) | -1 | -1 |
| G: -6322.92103 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.95455 HOMO: -6.90081 LUMO: -2.64767 factor:1 | 1 (-0.66782) | -1 | -1 |
| G: -6322.92103 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.61090 HOMO: -6.93890 LUMO: -2.65039 factor:1 | 1 (-0.32417) | -1 | -1 |
| G: -6322.92103 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.66499 HOMO: -6.80013 LUMO: -2.54154 factor:1 | 1 (-0.37827) | -1 | -1 |
| G: -6322.92103 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.86538 HOMO: -6.68040 LUMO: -0.89798 factor:1 | 1 (-0.57865) | -1 | -1 |
| G: -6322.92103 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.86747 HOMO: -7.01782 LUMO: -1.09662 factor:1 | 1 (-0.58075) | -1 | -1 |
| G: -6322.92103 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.76527 HOMO: -6.58516 LUMO: -0.83539 factor:1 | 1 (-0.47854) | -1 | -1 |
| G: -6322.92103 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12588.05330 HOMO: -7.46953 LUMO: 0.06259 factor:1 | 1 (-0.76657) | 1 | 1 |
| G: -6322.92103 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.67560 HOMO: -6.96884 LUMO: -0.99866 factor:1 | 1 (-0.38888) | -1 | -1 |
| G: -6322.92103 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.47318 HOMO: -7.29809 LUMO: -0.19320 factor:1 | 1 (-0.18645) | 1 | 1 |
| G: -6322.92103 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.61928 HOMO: -6.86271 LUMO: 0.04082 factor:1 | 1 (-0.33255) | -1 | -1 |
| G: -6322.92103 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.67305 HOMO: -6.36746 LUMO: -1.02587 factor:1 | 1 (-0.38632) | -1 | -1 |
| G: -6322.92103 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.66535 HOMO: -7.15659 LUMO: -1.25989 factor:1 | 1 (-0.37862) | 1 | 1 |
| G: -6322.92103 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.56717 HOMO: -6.69128 LUMO: -0.59865 factor:1 | 1 (-0.28044) | -1 | -1 |
| G: -6322.92103 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.44978 HOMO: -7.09129 LUMO: -1.08573 factor:1 | 1 (-0.16305) | 1 | 1 |
| G: -6322.92103 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.25987 HOMO: -6.64502 LUMO: -0.66396 factor:1 | -1 (0.02686) | -1 | -1 |
| G: -6322.92103 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.42795 HOMO: -6.93346 LUMO: -0.87349 factor:1 | 1 (-0.14123) | -1 | -1 |
| G: -6322.92103 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12588.04734 HOMO: -6.77019 LUMO: -0.87349 factor:1 | 1 (-0.76061) | -1 | -1 |
| G: -6322.92103 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.75074 HOMO: -6.59060 LUMO: -0.82995 factor:1 | 1 (-0.46401) | -1 | -1 |
| G: -6322.92103 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.73574 HOMO: -7.17564 LUMO: -1.08846 factor:1 | 1 (-0.44902) | 1 | 1 |
| G: -6322.92103 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.98834 HOMO: -7.27088 LUMO: -1.18642 factor:1 | 1 (-0.70162) | 1 | 1 |
| G: -6322.92103 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.66102 HOMO: -7.06680 LUMO: -1.13199 factor:1 | 1 (-0.37429) | 1 | 1 |
| G: -6322.92103 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.83457 HOMO: -7.21918 LUMO: -1.03947 factor:1 | 1 (-0.54785) | 1 | 1 |
| G: -6322.92103 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.92976 HOMO: -7.26000 LUMO: -0.11973 factor:1 | 1 (-0.64303) | 1 | 1 |
| G: -6322.92103 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.78118 HOMO: -6.77564 LUMO: 0.23402 factor:1 | 1 (-0.49446) | -1 | -1 |
| G: -6322.92103 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.50357 HOMO: -7.07224 LUMO: -0.75648 factor:1 | 1 (-0.21685) | 1 | 1 |
| G: -6322.92103 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.41321 HOMO: -7.45048 LUMO: 0.18232 factor:1 | 1 (-0.12648) | 1 | 1 |
| G: -6322.92103 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.73063 HOMO: -7.48313 LUMO: 0.15238 factor:1 | 1 (-0.44390) | 1 | 1 |
| G: -6322.92103 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.59851 HOMO: -6.60692 LUMO: -0.50885 factor:1 | 1 (-0.31179) | -1 | -1 |
| G: -6322.92103 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.74622 HOMO: -6.62869 LUMO: -0.60954 factor:1 | 1 (-0.45949) | -1 | -1 |
| G: -6322.92103 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.70526 HOMO: -7.40422 LUMO: -1.28982 factor:1 | 1 (-0.41854) | 1 | 1 |
| G: -6322.92103 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.59541 HOMO: -6.75114 LUMO: -1.23268 factor:1 | 1 (-0.30869) | -1 | -1 |
| G: -6322.92103 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.94924 HOMO: -6.84638 LUMO: -0.73199 factor:1 | 1 (-0.66252) | -1 | -1 |
| G: -6322.92103 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.73642 HOMO: -6.79196 LUMO: -1.43676 factor:1 | 1 (-0.44970) | -1 | -1 |
| G: -6322.92103 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.66611 HOMO: -7.00965 LUMO: -1.37690 factor:1 | 1 (-0.37938) | -1 | -1 |
| G: -6322.92103 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.60837 HOMO: -6.97972 LUMO: -1.58098 factor:1 | 1 (-0.32164) | -1 | -1 |
| G: -6322.92103 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.43944 HOMO: -6.91169 LUMO: -1.48574 factor:1 | 1 (-0.15271) | -1 | -1 |
| G: -6322.92103 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.51274 HOMO: -6.90081 LUMO: -1.30343 factor:1 | 1 (-0.22602) | -1 | -1 |
| G: -6322.92103 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.68897 HOMO: -6.78652 LUMO: -1.51840 factor:1 | 1 (-0.40224) | -1 | -1 |
| G: -6322.92103 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.72317 HOMO: -6.84638 LUMO: -1.15104 factor:1 | 1 (-0.43644) | -1 | -1 |
| G: -6322.92103 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.83591 HOMO: -6.61237 LUMO: -0.89798 factor:1 | 1 (-0.54918) | -1 | -1 |
| G: -6322.92103 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.56306 HOMO: -7.16204 LUMO: -1.30070 factor:1 | 1 (-0.27633) | 1 | 1 |
| G: -6322.92103 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.43650 HOMO: -7.32803 LUMO: 0.14694 factor:1 | 1 (-0.14977) | 1 | 1 |
| G: -6322.92103 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.40510 HOMO: -6.99877 LUMO: -0.87621 factor:1 | 1 (-0.11837) | -1 | -1 |
| G: -6322.92103 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.20942 HOMO: -6.99877 LUMO: -0.97145 factor:1 | -1 (0.07731) | -1 | -1 |
| G: -6322.92103 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.86867 HOMO: -7.08040 LUMO: -1.09662 factor:1 | 1 (-0.58194) | 1 | 1 |
| G: -6322.92103 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.75710 HOMO: -6.90897 LUMO: -1.14016 factor:1 | 1 (-0.47038) | -1 | -1 |
| G: -6322.92103 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.63536 HOMO: -6.68312 LUMO: -0.74831 factor:1 | 1 (-0.34863) | -1 | -1 |
| G: -6322.92103 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.64581 HOMO: -6.99061 LUMO: -0.86804 factor:1 | 1 (-0.35908) | -1 | -1 |
| G: -6322.92103 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.80742 HOMO: -7.10761 LUMO: -1.18642 factor:1 | 1 (-0.52069) | 1 | 1 |
| G: -6322.92103 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.69180 HOMO: -6.79196 LUMO: -0.71294 factor:1 | 1 (-0.40507) | -1 | -1 |
| G: -6322.92103 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.89811 HOMO: -6.86271 LUMO: -0.81362 factor:1 | 1 (-0.61139) | -1 | -1 |
| G: -6322.92103 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.84276 HOMO: -7.01510 LUMO: -0.99322 factor:1 | 1 (-0.55604) | -1 | -1 |
| G: -6322.92103 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.61158 HOMO: -6.88720 LUMO: -0.87893 factor:1 | 1 (-0.32485) | -1 | -1 |
| G: -6322.92103 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.52845 HOMO: -6.88448 LUMO: 0.22041 factor:1 | 1 (-0.24172) | -1 | -1 |
| G: -6322.92103 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.53468 HOMO: -7.55932 LUMO: 1.12111 factor:1 | 1 (-0.24795) | 1 | 1 |
| G: -6322.92103 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.42469 HOMO: -6.46815 LUMO: -0.86260 factor:1 | 1 (-0.13796) | -1 | -1 |
| G: -6322.92103 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.94908 HOMO: -7.13755 LUMO: 0.23130 factor:1 | 1 (-0.66235) | 1 | 1 |
| G: -6322.92103 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.71463 HOMO: -6.78924 LUMO: 1.51023 factor:1 | 1 (-0.42790) | -1 | -1 |
| G: -6322.92103 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.59819 HOMO: -6.48992 LUMO: 1.74969 factor:1 | 1 (-0.31146) | -1 | -1 |
| G: -6322.92103 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.76663 HOMO: -6.78380 LUMO: 1.81500 factor:1 | 1 (-0.47990) | -1 | -1 |
| G: -6322.92103 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.47653 HOMO: -6.49536 LUMO: 1.70615 factor:1 | 1 (-0.18980) | -1 | -1 |
| G: -6322.92103 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.49057 HOMO: -6.38651 LUMO: 1.44492 factor:1 | 1 (-0.20384) | -1 | -1 |
| G: -6322.92103 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.34504 HOMO: -6.83822 LUMO: 1.38234 factor:1 | 1 (-0.05831) | -1 | -1 |
| G: -6322.92103 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.61500 HOMO: -6.01644 LUMO: 1.20274 factor:1 | 1 (-0.32828) | -1 | -1 |
| G: -6322.92103 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.33919 HOMO: -6.18243 LUMO: 1.77962 factor:1 | 1 (-0.05246) | -1 | -1 |
| G: -6322.92103 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.33650 HOMO: -6.81917 LUMO: -1.01771 factor:1 | 1 (-0.04977) | -1 | -1 |
| G: -6322.92103 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.19353 HOMO: -6.61237 LUMO: -0.91702 factor:1 | -1 (0.09320) | -1 | -1 |
| G: -6322.92103 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.33541 HOMO: -6.84094 LUMO: -0.84900 factor:1 | 1 (-0.04868) | -1 | -1 |
| G: -6322.92103 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.20477 HOMO: -6.81917 LUMO: -1.01771 factor:1 | -1 (0.08196) | -1 | -1 |
| G: -6322.92103 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12586.96528 HOMO: -7.86953 LUMO: 1.16737 factor:1 | -1 (0.32145) | 1 | 1 |
| G: -6322.92103 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.44295 HOMO: -7.40694 LUMO: 0.11429 factor:1 | 1 (-0.15622) | 1 | 1 |
| G: -6322.92103 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.64031 HOMO: -6.70489 LUMO: -0.65035 factor:1 | 1 (-0.35358) | -1 | -1 |
| G: -6322.92103 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.83196 HOMO: -7.23279 LUMO: 0.33470 factor:1 | 1 (-0.54523) | 1 | 1 |
| G: -6322.92103 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.81838 HOMO: -7.17020 LUMO: 0.41361 factor:1 | 1 (-0.53166) | 1 | 1 |
| G: -6322.92103 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.61079 HOMO: -6.90353 LUMO: -0.90070 factor:1 | 1 (-0.32406) | -1 | -1 |
| G: -6322.92103 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.80676 HOMO: -7.39061 LUMO: 0.17687 factor:1 | 1 (-0.52004) | 1 | 1 |
| G: -6322.92103 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.81397 HOMO: -7.16748 LUMO: 0.42178 factor:1 | 1 (-0.52725) | 1 | 1 |
| G: -6322.92103 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.91980 HOMO: -7.36884 LUMO: -1.11295 factor:1 | 1 (-0.63307) | 1 | 1 |
| G: -6322.92103 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.69683 HOMO: -7.33347 LUMO: 0.33198 factor:1 | 1 (-0.41010) | 1 | 1 |
| G: -6322.92103 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.61838 HOMO: -7.31986 LUMO: -0.83539 factor:1 | 1 (-0.33165) | 1 | 1 |
| G: -6322.92103 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.60265 HOMO: -7.31170 LUMO: 0.08708 factor:1 | 1 (-0.31592) | 1 | 1 |
| G: -6322.92103 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.46610 HOMO: -7.36884 LUMO: 0.38096 factor:1 | 1 (-0.17938) | 1 | 1 |
| G: -6322.92103 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.39862 HOMO: -6.99333 LUMO: 1.74153 factor:1 | 1 (-0.11189) | -1 | -1 |
| G: -6322.92103 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.45351 HOMO: -6.94435 LUMO: 1.74969 factor:1 | 1 (-0.16678) | -1 | -1 |
| G: -6322.92103 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.47688 HOMO: -7.02598 LUMO: 1.43404 factor:1 | 1 (-0.19015) | -1 | -1 |
| G: -6322.92103 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.38599 HOMO: -6.41100 LUMO: 1.62996 factor:1 | 1 (-0.09927) | -1 | -1 |
| G: -6322.92103 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.67033 HOMO: -6.57699 LUMO: 1.81228 factor:1 | 1 (-0.38360) | -1 | -1 |
| G: -6322.92103 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.66442 HOMO: -6.86543 LUMO: 1.49935 factor:1 | 1 (-0.37769) | -1 | -1 |
| G: -6322.92103 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.67767 HOMO: -6.91169 LUMO: -1.22451 factor:1 | 1 (-0.39095) | -1 | -1 |
| G: -6322.92103 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.59743 HOMO: -7.09945 LUMO: -1.23812 factor:1 | 1 (-0.31070) | 1 | 1 |
| G: -6322.92103 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.35639 HOMO: -7.48857 LUMO: 0.10340 factor:1 | 1 (-0.06966) | 1 | 1 |
| G: -6322.92103 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.45541 HOMO: -7.21918 LUMO: -0.06803 factor:1 | 1 (-0.16868) | 1 | 1 |
| G: -6322.92103 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.39625 HOMO: -6.34025 LUMO: -0.68845 factor:1 | 1 (-0.10953) | -1 | -1 |
| G: -6322.92103 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.25522 HOMO: -6.82734 LUMO: -0.77825 factor:1 | -1 (0.03151) | -1 | -1 |
| G: -6322.92103 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.51952 HOMO: -6.92258 LUMO: -1.03675 factor:1 | 1 (-0.23279) | -1 | -1 |
| G: -6322.92103 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.83389 HOMO: -6.42461 LUMO: -0.95240 factor:1 | 1 (-0.54717) | -1 | -1 |
| G: -6322.92103 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.53892 HOMO: -6.96067 LUMO: -1.05036 factor:1 | 1 (-0.25220) | -1 | -1 |
| G: -6322.92103 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.59070 HOMO: -7.23551 LUMO: 0.12245 factor:1 | 1 (-0.30398) | 1 | 1 |
| G: -6322.92103 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.66608 HOMO: -6.85183 LUMO: 0.16055 factor:1 | 1 (-0.37935) | -1 | -1 |
| G: -6322.92103 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.74687 HOMO: -6.46815 LUMO: -0.89253 factor:1 | 1 (-0.46014) | -1 | -1 |
| G: -6322.92103 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.70246 HOMO: -7.23823 LUMO: -0.06259 factor:1 | 1 (-0.41574) | 1 | 1 |
| G: -6322.92103 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.38719 HOMO: -6.76475 LUMO: -0.99049 factor:1 | 1 (-0.10046) | -1 | -1 |
| G: -6322.92103 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.54673 HOMO: -7.14843 LUMO: -0.88165 factor:1 | 1 (-0.26000) | 1 | 1 |
| G: -6322.92103 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.38009 HOMO: -7.15659 LUMO: 0.20681 factor:1 | 1 (-0.09336) | 1 | 1 |
| G: -6322.92103 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.74995 HOMO: -7.11306 LUMO: 0.14150 factor:1 | 1 (-0.46322) | 1 | 1 |
| G: -6322.92103 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.69033 HOMO: -6.67223 LUMO: -0.86260 factor:1 | 1 (-0.40360) | -1 | -1 |
| G: -6322.92103 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.63841 HOMO: -6.92530 LUMO: 0.30749 factor:1 | 1 (-0.35168) | -1 | -1 |
| G: -6322.92103 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.36512 HOMO: -6.50624 LUMO: -0.70477 factor:1 | 1 (-0.07840) | -1 | -1 |
| G: -6322.92103 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.43827 HOMO: -7.35524 LUMO: 0.75103 factor:1 | 1 (-0.15154) | 1 | 1 |
| G: -6322.92103 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.30986 HOMO: -7.07768 LUMO: -0.26939 factor:1 | 1 (-0.02313) | 1 | 1 |
| G: -6322.92103 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.19628 HOMO: -7.15932 LUMO: 0.42450 factor:1 | -1 (0.09045) | 1 | 1 |
| G: -6322.92103 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12586.98457 HOMO: -7.46136 LUMO: 0.04626 factor:1 | -1 (0.30216) | 1 | 1 |
| G: -6322.92103 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.52787 HOMO: -7.05047 LUMO: -1.06669 factor:1 | 1 (-0.24115) | -1 | -1 |
| G: -6322.92103 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.40319 HOMO: -6.66951 LUMO: -0.99322 factor:1 | 1 (-0.11646) | -1 | -1 |
| G: -6323.75087 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12588.02195 HOMO: -7.01782 LUMO: -1.08846 factor:1 | -1 (0.09461) | -1 | -1 |
| G: -6323.75087 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12588.08797 HOMO: -7.03959 LUMO: -1.15376 factor:1 | -1 (0.02860) | -1 | -1 |
| G: -6323.75087 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12588.15719 HOMO: -6.68856 LUMO: 1.61364 factor:1 | 1 (-0.04063) | -1 | -1 |
| G: -6323.75087 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.78918 HOMO: -6.53345 LUMO: 1.60275 factor:1 | -1 (0.32738) | -1 | -1 |
| G: -6323.75087 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.85993 HOMO: -6.73482 LUMO: 1.86398 factor:1 | -1 (0.25663) | -1 | -1 |
| G: -6323.75087 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.69441 HOMO: -6.87632 LUMO: 1.59731 factor:1 | -1 (0.42216) | -1 | -1 |
| G: -6323.75087 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12588.07695 HOMO: -6.31848 LUMO: 2.12521 factor:1 | -1 (0.03962) | -1 | -1 |
| G: -6323.75087 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12588.08105 HOMO: -6.35114 LUMO: 1.71432 factor:1 | -1 (0.03551) | -1 | -1 |
| G: -6323.75087 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.76791 HOMO: -6.34842 LUMO: 1.92929 factor:1 | -1 (0.34866) | -1 | -1 |
| G: -6323.75087 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.67101 HOMO: -6.14977 LUMO: 1.78235 factor:1 | -1 (0.44556) | -1 | -1 |
| G: -6323.75087 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.88989 HOMO: -6.31032 LUMO: 1.51567 factor:1 | -1 (0.22667) | -1 | -1 |
| G: -6323.75087 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.50722 HOMO: -6.25862 LUMO: 1.75241 factor:1 | -1 (0.60934) | -1 | -1 |
| G: -6323.75087 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.67724 HOMO: -6.49264 LUMO: 1.66806 factor:1 | -1 (0.43933) | -1 | -1 |
| G: -6323.75087 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.71941 HOMO: -6.28311 LUMO: 1.60003 factor:1 | -1 (0.39715) | -1 | -1 |
| G: -6323.75087 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.84644 HOMO: -7.13210 LUMO: -0.04354 factor:1 | -1 (0.27013) | 1 | 1 |
| G: -6323.75087 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.95455 HOMO: -7.35252 LUMO: 0.03537 factor:1 | -1 (0.16202) | 1 | 1 |
| G: -6323.75087 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.61090 HOMO: -6.58243 LUMO: -0.48980 factor:1 | -1 (0.50567) | -1 | -1 |
| G: -6323.75087 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.66499 HOMO: -6.90081 LUMO: -0.05442 factor:1 | -1 (0.45157) | -1 | -1 |
| G: -6323.75087 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.86538 HOMO: -7.22734 LUMO: 0.17143 factor:1 | -1 (0.25119) | 1 | 1 |
| G: -6323.75087 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.86747 HOMO: -7.13210 LUMO: -0.99866 factor:1 | -1 (0.24909) | 1 | 1 |
| G: -6323.75087 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.76527 HOMO: -7.39878 LUMO: 0.13334 factor:1 | -1 (0.35130) | 1 | 1 |
| G: -6323.75087 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12588.05330 HOMO: -7.04503 LUMO: -0.89798 factor:1 | -1 (0.06327) | -1 | -1 |
| G: -6323.75087 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.67560 HOMO: -6.95523 LUMO: -1.07213 factor:1 | -1 (0.44096) | -1 | -1 |
| G: -6323.75087 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.47318 HOMO: -6.75114 LUMO: -1.28438 factor:1 | -1 (0.64339) | -1 | -1 |
| G: -6323.75087 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.61928 HOMO: -6.75114 LUMO: -0.11701 factor:1 | -1 (0.49729) | -1 | -1 |
| G: -6323.75087 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.67305 HOMO: -6.83278 LUMO: -0.01633 factor:1 | -1 (0.44352) | -1 | -1 |
| G: -6323.75087 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.66535 HOMO: -6.93890 LUMO: -0.88981 factor:1 | -1 (0.45122) | -1 | -1 |
| G: -6323.75087 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.56717 HOMO: -7.07224 LUMO: -1.08573 factor:1 | -1 (0.54940) | 1 | 1 |
| G: -6323.75087 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.44978 HOMO: -6.99877 LUMO: -0.95240 factor:1 | -1 (0.66679) | -1 | -1 |
| G: -6323.75087 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.25987 HOMO: -7.09129 LUMO: 0.35375 factor:1 | -1 (0.85670) | 1 | 1 |
| G: -6323.75087 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.42795 HOMO: -7.09401 LUMO: 0.04354 factor:1 | -1 (0.68861) | 1 | 1 |
| G: -6323.75087 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12588.04734 HOMO: -6.85183 LUMO: -0.68573 factor:1 | -1 (0.06923) | -1 | -1 |
| G: -6323.75087 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.75074 HOMO: -6.83006 LUMO: -0.58777 factor:1 | -1 (0.36583) | -1 | -1 |
| G: -6323.75087 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.73574 HOMO: -7.40422 LUMO: 0.17687 factor:1 | -1 (0.38082) | 1 | 1 |
| G: -6323.75087 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.98834 HOMO: -7.15932 LUMO: 0.10340 factor:1 | -1 (0.12822) | 1 | 1 |
| G: -6323.75087 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.66102 HOMO: -7.03414 LUMO: -0.19592 factor:1 | -1 (0.45555) | -1 | -1 |
| G: -6323.75087 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.83457 HOMO: -6.48447 LUMO: -0.36191 factor:1 | -1 (0.28199) | -1 | -1 |
| G: -6323.75087 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.92976 HOMO: -7.49402 LUMO: 0.11429 factor:1 | -1 (0.18681) | 1 | 1 |
| G: -6323.75087 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.78118 HOMO: -7.01237 LUMO: -1.06397 factor:1 | -1 (0.33538) | -1 | -1 |
| G: -6323.75087 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.50357 HOMO: -6.67223 LUMO: -1.07213 factor:1 | -1 (0.61299) | -1 | -1 |
| G: -6323.75087 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.41321 HOMO: -7.38789 LUMO: -1.15376 factor:1 | -1 (0.70336) | 1 | 1 |
| G: -6323.75087 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.73063 HOMO: -6.42461 LUMO: -1.23812 factor:1 | -1 (0.38594) | -1 | -1 |
| G: -6323.75087 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.59851 HOMO: -7.36884 LUMO: -1.19186 factor:1 | -1 (0.51805) | 1 | 1 |
| G: -6323.75087 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.74622 HOMO: -6.65591 LUMO: 0.07075 factor:1 | -1 (0.37035) | -1 | -1 |
| G: -6323.75087 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.70526 HOMO: -7.39061 LUMO: -0.16871 factor:1 | -1 (0.41130) | 1 | 1 |
| G: -6323.75087 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.59541 HOMO: -6.90353 LUMO: -0.96056 factor:1 | -1 (0.52115) | -1 | -1 |
| G: -6323.75087 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.94924 HOMO: -7.42054 LUMO: 0.19048 factor:1 | -1 (0.16732) | 1 | 1 |
| G: -6323.75087 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.73642 HOMO: -7.40150 LUMO: 0.35647 factor:1 | -1 (0.38014) | 1 | 1 |
| G: -6323.75087 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.66611 HOMO: -6.56067 LUMO: -0.96056 factor:1 | -1 (0.45046) | -1 | -1 |
| G: -6323.75087 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.60837 HOMO: -6.89809 LUMO: -0.81090 factor:1 | -1 (0.50820) | -1 | -1 |
| G: -6323.75087 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.43944 HOMO: -6.91986 LUMO: -0.84900 factor:1 | -1 (0.67713) | -1 | -1 |
| G: -6323.75087 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.51274 HOMO: -6.61509 LUMO: -0.62042 factor:1 | -1 (0.60382) | -1 | -1 |
| G: -6323.75087 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.68897 HOMO: -6.58243 LUMO: -0.65579 factor:1 | -1 (0.42760) | -1 | -1 |
| G: -6323.75087 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.72317 HOMO: -6.52257 LUMO: -0.92519 factor:1 | -1 (0.39340) | -1 | -1 |
| G: -6323.75087 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.83591 HOMO: -6.69128 LUMO: 1.49118 factor:1 | -1 (0.28066) | -1 | -1 |
| G: -6323.75087 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.56306 HOMO: -7.02870 LUMO: 1.67894 factor:1 | -1 (0.55351) | -1 | -1 |
| G: -6323.75087 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.43650 HOMO: -6.88720 LUMO: 1.68711 factor:1 | -1 (0.68007) | -1 | -1 |
| G: -6323.75087 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.40510 HOMO: -5.89943 LUMO: 1.03675 factor:1 | -1 (0.71147) | -1 | -1 |
| G: -6323.75087 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.20942 HOMO: -6.40556 LUMO: 1.14560 factor:1 | -1 (0.90715) | -1 | -1 |
| G: -6323.75087 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.86867 HOMO: -6.51168 LUMO: 1.48030 factor:1 | -1 (0.24790) | -1 | -1 |
| G: -6323.75087 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.75710 HOMO: -6.64502 LUMO: 1.91568 factor:1 | -1 (0.35946) | -1 | -1 |
| G: -6323.75087 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.63536 HOMO: -6.47903 LUMO: 1.91296 factor:1 | -1 (0.48121) | -1 | -1 |
| G: -6323.75087 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.64581 HOMO: -6.34297 LUMO: 1.91840 factor:1 | -1 (0.47076) | -1 | -1 |
| G: -6323.75087 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.80742 HOMO: -6.89809 LUMO: 1.82861 factor:1 | -1 (0.30915) | -1 | -1 |
| G: -6323.75087 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.69180 HOMO: -6.10079 LUMO: 1.62996 factor:1 | -1 (0.42477) | -1 | -1 |
| G: -6323.75087 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.89811 HOMO: -7.16476 LUMO: -0.92247 factor:1 | -1 (0.21845) | 1 | 1 |
| G: -6323.75087 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.84276 HOMO: -7.10489 LUMO: -0.95784 factor:1 | -1 (0.27380) | 1 | 1 |
| G: -6323.75087 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.61158 HOMO: -6.76475 LUMO: -0.99866 factor:1 | -1 (0.50499) | -1 | -1 |
| G: -6323.75087 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.52845 HOMO: -6.81373 LUMO: -1.05036 factor:1 | -1 (0.58812) | -1 | -1 |
| G: -6323.75087 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.53468 HOMO: -6.90081 LUMO: -1.03947 factor:1 | -1 (0.58189) | -1 | -1 |
| G: -6323.75087 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.42469 HOMO: -7.06952 LUMO: -0.91702 factor:1 | -1 (0.69188) | 1 | 1 |
| G: -6323.75087 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.94908 HOMO: -6.73482 LUMO: -0.94151 factor:1 | -1 (0.16749) | -1 | -1 |
| G: -6323.75087 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.71463 HOMO: -6.99605 LUMO: -1.04764 factor:1 | -1 (0.40194) | -1 | -1 |
| G: -6323.75087 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.59819 HOMO: -7.03686 LUMO: -0.93335 factor:1 | -1 (0.51838) | -1 | -1 |
| G: -6323.75087 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.76663 HOMO: -6.81101 LUMO: -0.95240 factor:1 | -1 (0.34994) | -1 | -1 |
| G: -6323.75087 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.47653 HOMO: -6.83822 LUMO: -0.65307 factor:1 | -1 (0.64004) | -1 | -1 |
| G: -6323.75087 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.49057 HOMO: -7.05319 LUMO: -0.81634 factor:1 | -1 (0.62600) | -1 | -1 |
| G: -6323.75087 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.34504 HOMO: -7.57565 LUMO: 0.19048 factor:1 | -1 (0.77152) | 1 | 1 |
| G: -6323.75087 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.61500 HOMO: -6.56067 LUMO: -0.50613 factor:1 | -1 (0.50156) | -1 | -1 |
| G: -6323.75087 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.33919 HOMO: -6.74298 LUMO: -0.70477 factor:1 | -1 (0.77737) | -1 | -1 |
| G: -6323.75087 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.33650 HOMO: -7.02054 LUMO: 0.03537 factor:1 | -1 (0.78007) | -1 | -1 |
| G: -6323.75087 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.19353 HOMO: -7.33347 LUMO: -0.17960 factor:1 | -1 (0.92304) | 1 | 1 |
| G: -6323.75087 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.33541 HOMO: -6.98244 LUMO: -0.88165 factor:1 | -1 (0.78116) | -1 | -1 |
| G: -6323.75087 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.20477 HOMO: -7.14843 LUMO: -1.19730 factor:1 | -1 (0.91180) | 1 | 1 |
| G: -6323.75087 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12586.96528 HOMO: -7.17564 LUMO: -1.21907 factor:1 | -1 (1.15129) | 1 | 1 |
| G: -6323.75087 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.44295 HOMO: -6.74026 LUMO: -0.86532 factor:1 | -1 (0.67362) | -1 | -1 |
| G: -6323.75087 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.64031 HOMO: -6.82462 LUMO: -1.24084 factor:1 | -1 (0.47625) | -1 | -1 |
| G: -6323.75087 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.83196 HOMO: -6.78924 LUMO: -0.70477 factor:1 | -1 (0.28460) | -1 | -1 |
| G: -6323.75087 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.81838 HOMO: -7.41238 LUMO: 0.05987 factor:1 | -1 (0.29818) | 1 | 1 |
| G: -6323.75087 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.61079 HOMO: -6.75931 LUMO: 0.02721 factor:1 | -1 (0.50578) | -1 | -1 |
| G: -6323.75087 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.80676 HOMO: -6.28583 LUMO: -0.93063 factor:1 | -1 (0.30980) | -1 | -1 |
| G: -6323.75087 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.81397 HOMO: -6.69128 LUMO: -0.83539 factor:1 | -1 (0.30259) | -1 | -1 |
| G: -6323.75087 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.91980 HOMO: -7.22190 LUMO: 0.01361 factor:1 | -1 (0.19677) | 1 | 1 |
| G: -6323.75087 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.69683 HOMO: -6.95251 LUMO: -1.09934 factor:1 | -1 (0.41974) | -1 | -1 |
| G: -6323.75087 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.61838 HOMO: -6.75387 LUMO: -0.90614 factor:1 | -1 (0.49819) | -1 | -1 |
| G: -6323.75087 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.60265 HOMO: -7.48585 LUMO: 0.05987 factor:1 | -1 (0.51391) | 1 | 1 |
| G: -6323.75087 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.46610 HOMO: -6.92802 LUMO: -0.66940 factor:1 | -1 (0.65046) | -1 | -1 |
| G: -6323.75087 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.39862 HOMO: -7.29537 LUMO: -0.14150 factor:1 | -1 (0.71795) | 1 | 1 |
| G: -6323.75087 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.45351 HOMO: -6.57155 LUMO: -0.86804 factor:1 | -1 (0.66306) | -1 | -1 |
| G: -6323.75087 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.47688 HOMO: -6.87632 LUMO: -0.77825 factor:1 | -1 (0.63969) | -1 | -1 |
| G: -6323.75087 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.38599 HOMO: -6.45998 LUMO: -0.31565 factor:1 | -1 (0.73057) | -1 | -1 |
| G: -6323.75087 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.67033 HOMO: -7.51306 LUMO: 0.05714 factor:1 | -1 (0.44624) | 1 | 1 |
| G: -6323.75087 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.66442 HOMO: -6.86271 LUMO: -0.00816 factor:1 | -1 (0.45214) | -1 | -1 |
| G: -6323.75087 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.67767 HOMO: -6.43277 LUMO: -1.07485 factor:1 | -1 (0.43889) | -1 | -1 |
| G: -6323.75087 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.59743 HOMO: -6.78108 LUMO: -0.81362 factor:1 | -1 (0.51914) | -1 | -1 |
| G: -6323.75087 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.35639 HOMO: -6.88448 LUMO: 1.21907 factor:1 | -1 (0.76018) | -1 | -1 |
| G: -6323.75087 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.45541 HOMO: -6.97700 LUMO: 1.44765 factor:1 | -1 (0.66116) | -1 | -1 |
| G: -6323.75087 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.39625 HOMO: -6.89537 LUMO: 2.12249 factor:1 | -1 (0.72031) | -1 | -1 |
| G: -6323.75087 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.25522 HOMO: -6.28311 LUMO: 1.45037 factor:1 | -1 (0.86135) | -1 | -1 |
| G: -6323.75087 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.51952 HOMO: -6.55522 LUMO: 1.39867 factor:1 | -1 (0.59705) | -1 | -1 |
| G: -6323.75087 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.83389 HOMO: -6.46815 LUMO: 1.50207 factor:1 | -1 (0.28267) | -1 | -1 |
| G: -6323.75087 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.53892 HOMO: -6.43549 LUMO: 2.17419 factor:1 | -1 (0.57764) | -1 | -1 |
| G: -6323.75087 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.59070 HOMO: -6.99333 LUMO: 1.87214 factor:1 | -1 (0.52586) | -1 | -1 |
| G: -6323.75087 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.66608 HOMO: -6.65591 LUMO: 1.37962 factor:1 | -1 (0.45048) | -1 | -1 |
| G: -6323.75087 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.74687 HOMO: -6.82734 LUMO: 1.55649 factor:1 | -1 (0.36969) | -1 | -1 |
| G: -6323.75087 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.70246 HOMO: -6.71849 LUMO: 1.36057 factor:1 | -1 (0.41410) | -1 | -1 |
| G: -6323.75087 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.38719 HOMO: -6.79468 LUMO: 1.82044 factor:1 | -1 (0.72937) | -1 | -1 |
| G: -6323.75087 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.54673 HOMO: -6.61237 LUMO: 1.15104 factor:1 | -1 (0.56983) | -1 | -1 |
| G: -6323.75087 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.38009 HOMO: -6.62053 LUMO: 2.33474 factor:1 | -1 (0.73648) | -1 | -1 |
| G: -6323.75087 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.74995 HOMO: -6.55794 LUMO: 1.65717 factor:1 | -1 (0.36662) | -1 | -1 |
| G: -6323.75087 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.69033 HOMO: -6.85999 LUMO: 2.03813 factor:1 | -1 (0.42624) | -1 | -1 |
| G: -6323.75087 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.63841 HOMO: -6.45726 LUMO: 1.28438 factor:1 | -1 (0.47816) | -1 | -1 |
| G: -6323.75087 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.36512 HOMO: -6.23685 LUMO: 1.93201 factor:1 | -1 (0.75144) | -1 | -1 |
| G: -6323.75087 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.43827 HOMO: -7.06680 LUMO: 1.86942 factor:1 | -1 (0.67830) | 1 | 1 |
| G: -6323.75087 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.30986 HOMO: -6.89537 LUMO: 2.17147 factor:1 | -1 (0.80671) | -1 | -1 |
| G: -6323.75087 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.19628 HOMO: -6.80013 LUMO: 1.78779 factor:1 | -1 (0.92029) | -1 | -1 |
| G: -6323.75087 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12586.98457 HOMO: -6.45726 LUMO: 1.58370 factor:1 | -1 (1.13199) | -1 | -1 |
| G: -6323.75087 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.52787 HOMO: -6.52529 LUMO: 1.71976 factor:1 | -1 (0.58869) | -1 | -1 |
| G: -6323.75087 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.40319 HOMO: -7.22462 LUMO: -1.18642 factor:1 | -1 (0.71337) | 1 | 1 |
| G: -6322.75232 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12588.02195 HOMO: -7.18381 LUMO: -0.78641 factor:1 | 1 (-0.90394) | 1 | 1 |
| G: -6322.75232 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12588.08797 HOMO: -6.93346 LUMO: 1.65717 factor:1 | 1 (-0.96995) | -1 | -1 |
| G: -6322.75232 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12588.15719 HOMO: -6.41644 LUMO: 1.78235 factor:1 | 1 (-1.03918) | -1 | -1 |
| G: -6322.75232 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.78918 HOMO: -6.59876 LUMO: 1.83677 factor:1 | 1 (-0.67117) | -1 | -1 |
| G: -6322.75232 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.85993 HOMO: -6.35658 LUMO: 1.59731 factor:1 | 1 (-0.74192) | -1 | -1 |
| G: -6322.75232 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.69441 HOMO: -6.60692 LUMO: 1.66534 factor:1 | 1 (-0.57639) | -1 | -1 |
| G: -6322.75232 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12588.07695 HOMO: -6.83006 LUMO: 2.11705 factor:1 | 1 (-0.95893) | -1 | -1 |
| G: -6322.75232 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12588.08105 HOMO: -6.89264 LUMO: 1.30070 factor:1 | 1 (-0.96304) | -1 | -1 |
| G: -6322.75232 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.76791 HOMO: -6.90081 LUMO: 2.05174 factor:1 | 1 (-0.64989) | -1 | -1 |
| G: -6322.75232 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.67101 HOMO: -6.74842 LUMO: 1.96194 factor:1 | 1 (-0.55299) | -1 | -1 |
| G: -6322.75232 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.88989 HOMO: -6.58516 LUMO: 1.30887 factor:1 | 1 (-0.77188) | -1 | -1 |
| G: -6322.75232 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.50722 HOMO: -7.00965 LUMO: 2.08167 factor:1 | 1 (-0.38920) | -1 | -1 |
| G: -6322.75232 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.67724 HOMO: -6.86815 LUMO: 2.29664 factor:1 | 1 (-0.55922) | -1 | -1 |
| G: -6322.75232 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.71941 HOMO: -6.39740 LUMO: 2.02725 factor:1 | 1 (-0.60140) | -1 | -1 |
| G: -6322.75232 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.84644 HOMO: -5.95929 LUMO: 1.62724 factor:1 | 1 (-0.72842) | -1 | -1 |
| G: -6322.75232 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.95455 HOMO: -6.71849 LUMO: 1.34696 factor:1 | 1 (-0.83653) | -1 | -1 |
| G: -6322.75232 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.61090 HOMO: -7.26816 LUMO: 1.74153 factor:1 | 1 (-0.49288) | 1 | 1 |
| G: -6322.75232 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.66499 HOMO: -6.90897 LUMO: 1.71432 factor:1 | 1 (-0.54698) | -1 | -1 |
| G: -6322.75232 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.86538 HOMO: -6.70489 LUMO: 1.91568 factor:1 | 1 (-0.74736) | -1 | -1 |
| G: -6322.75232 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.86747 HOMO: -6.83278 LUMO: 1.61908 factor:1 | 1 (-0.74946) | -1 | -1 |
| G: -6322.75232 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.76527 HOMO: -7.17292 LUMO: 1.95378 factor:1 | 1 (-0.64725) | 1 | -1 |
| G: -6322.75232 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12588.05330 HOMO: -6.53345 LUMO: 1.74153 factor:1 | 1 (-0.93528) | -1 | -1 |
| G: -6322.75232 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.67560 HOMO: -6.53073 LUMO: 1.51023 factor:1 | 1 (-0.55759) | -1 | -1 |
| G: -6322.75232 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.47318 HOMO: -6.93346 LUMO: 2.22861 factor:1 | 1 (-0.35516) | -1 | -1 |
| G: -6322.75232 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.61928 HOMO: -6.47903 LUMO: 2.05446 factor:1 | 1 (-0.50126) | -1 | -1 |
| G: -6322.75232 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.67305 HOMO: -6.88992 LUMO: 1.57010 factor:1 | 1 (-0.55503) | -1 | -1 |
| G: -6322.75232 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.66535 HOMO: -6.07358 LUMO: 1.95922 factor:1 | 1 (-0.54733) | -1 | -1 |
| G: -6322.75232 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.56717 HOMO: -6.75114 LUMO: 2.18780 factor:1 | 1 (-0.44915) | -1 | -1 |
| G: -6322.75232 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.44978 HOMO: -6.96339 LUMO: 1.70071 factor:1 | 1 (-0.33176) | -1 | -1 |
| G: -6322.75232 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.25987 HOMO: -7.14843 LUMO: 1.82588 factor:1 | 1 (-0.14185) | 1 | -1 |
| G: -6322.75232 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.42795 HOMO: -6.96339 LUMO: 2.29392 factor:1 | 1 (-0.30994) | -1 | -1 |
| G: -6322.75232 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12588.04734 HOMO: -6.81645 LUMO: 2.39732 factor:1 | 1 (-0.92932) | -1 | -1 |
| G: -6322.75232 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.75074 HOMO: -6.48447 LUMO: 1.24084 factor:1 | 1 (-0.63272) | -1 | -1 |
| G: -6322.75232 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.73574 HOMO: -7.14843 LUMO: 2.01092 factor:1 | 1 (-0.61773) | 1 | -1 |
| G: -6322.75232 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.98834 HOMO: -7.20013 LUMO: -0.34286 factor:1 | 1 (-0.87033) | 1 | -1 |
| G: -6322.75232 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.66102 HOMO: -6.97700 LUMO: -0.15238 factor:1 | 1 (-0.54300) | -1 | -1 |
| G: -6322.75232 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.83457 HOMO: -7.07768 LUMO: -0.26123 factor:1 | 1 (-0.71656) | 1 | -1 |
| G: -6322.75232 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.92976 HOMO: -6.99333 LUMO: -0.41361 factor:1 | 1 (-0.81174) | -1 | -1 |
| G: -6322.75232 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.78118 HOMO: -6.84638 LUMO: -0.40273 factor:1 | 1 (-0.66317) | -1 | -1 |
| G: -6322.75232 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.50357 HOMO: -6.83822 LUMO: -0.26939 factor:1 | 1 (-0.38556) | -1 | -1 |
| G: -6322.75232 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.41321 HOMO: -6.75931 LUMO: -0.93879 factor:1 | 1 (-0.29519) | -1 | -1 |
| G: -6322.75232 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.73063 HOMO: -6.79468 LUMO: -0.39729 factor:1 | 1 (-0.61261) | -1 | -1 |
| G: -6322.75232 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.59851 HOMO: -6.93890 LUMO: 0.43266 factor:1 | 1 (-0.48050) | -1 | -1 |
| G: -6322.75232 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.74622 HOMO: -7.08040 LUMO: -0.85716 factor:1 | 1 (-0.62820) | 1 | 1 |
| G: -6322.75232 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.70526 HOMO: -6.70216 LUMO: -1.41499 factor:1 | 1 (-0.58725) | -1 | -1 |
| G: -6322.75232 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.59541 HOMO: -6.63686 LUMO: -0.52790 factor:1 | 1 (-0.47740) | -1 | -1 |
| G: -6322.75232 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.94924 HOMO: -6.75114 LUMO: -0.13334 factor:1 | 1 (-0.83123) | -1 | -1 |
| G: -6322.75232 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.73642 HOMO: -6.94435 LUMO: -0.24490 factor:1 | 1 (-0.61841) | -1 | -1 |
| G: -6322.75232 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.66611 HOMO: -6.74298 LUMO: -0.84627 factor:1 | 1 (-0.54809) | -1 | -1 |
| G: -6322.75232 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.60837 HOMO: -7.15932 LUMO: 0.22041 factor:1 | 1 (-0.49035) | 1 | 1 |
| G: -6322.75232 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.43944 HOMO: -6.90081 LUMO: -1.16737 factor:1 | 1 (-0.32142) | -1 | -1 |
| G: -6322.75232 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.51274 HOMO: -7.04775 LUMO: -0.84355 factor:1 | 1 (-0.39473) | -1 | -1 |
| G: -6322.75232 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.68897 HOMO: -7.17020 LUMO: -1.31159 factor:1 | 1 (-0.57095) | 1 | 1 |
| G: -6322.75232 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.72317 HOMO: -7.14571 LUMO: -0.46259 factor:1 | 1 (-0.60515) | 1 | 1 |
| G: -6322.75232 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.83591 HOMO: -7.45048 LUMO: -0.91158 factor:1 | 1 (-0.71789) | 1 | 1 |
| G: -6322.75232 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.56306 HOMO: -6.87360 LUMO: -0.82995 factor:1 | 1 (-0.44504) | -1 | -1 |
| G: -6322.75232 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.43650 HOMO: -7.43415 LUMO: -0.65307 factor:1 | 1 (-0.31848) | 1 | 1 |
| G: -6322.75232 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.40510 HOMO: -7.47225 LUMO: -0.77280 factor:1 | 1 (-0.28708) | 1 | 1 |
| G: -6322.75232 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.20942 HOMO: -6.86271 LUMO: -0.83811 factor:1 | 1 (-0.09140) | -1 | -1 |
| G: -6322.75232 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.86867 HOMO: -7.53483 LUMO: -0.66124 factor:1 | 1 (-0.75065) | 1 | 1 |
| G: -6322.75232 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.75710 HOMO: -7.45864 LUMO: -1.08301 factor:1 | 1 (-0.63909) | 1 | 1 |
| G: -6322.75232 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.63536 HOMO: -7.24639 LUMO: -1.19186 factor:1 | 1 (-0.51734) | 1 | 1 |
| G: -6322.75232 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.64581 HOMO: -7.54844 LUMO: -0.96873 factor:1 | 1 (-0.52779) | 1 | 1 |
| G: -6322.75232 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.80742 HOMO: -7.12666 LUMO: -0.01633 factor:1 | 1 (-0.68940) | 1 | 1 |
| G: -6322.75232 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.69180 HOMO: -6.77291 LUMO: -0.70477 factor:1 | 1 (-0.57378) | -1 | -1 |
| G: -6322.75232 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.89811 HOMO: -6.76475 LUMO: -1.15921 factor:1 | 1 (-0.78010) | -1 | -1 |
| G: -6322.75232 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.84276 HOMO: -5.37697 LUMO: -0.56600 factor:1 | 1 (-0.72475) | -1 | -1 |
| G: -6322.75232 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.61158 HOMO: -6.62053 LUMO: -1.75513 factor:1 | 1 (-0.49356) | -1 | -1 |
| G: -6322.75232 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.52845 HOMO: -6.60420 LUMO: -1.74697 factor:1 | 1 (-0.41043) | -1 | -1 |
| G: -6322.75232 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.53468 HOMO: -6.84366 LUMO: -0.94968 factor:1 | 1 (-0.41666) | -1 | -1 |
| G: -6322.75232 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.42469 HOMO: -6.96884 LUMO: -2.11977 factor:1 | 1 (-0.30667) | -1 | -1 |
| G: -6322.75232 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.94908 HOMO: -6.80829 LUMO: 0.56055 factor:1 | 1 (-0.83106) | -1 | -1 |
| G: -6322.75232 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.71463 HOMO: -7.02326 LUMO: 0.11429 factor:1 | 1 (-0.59661) | -1 | -1 |
| G: -6322.75232 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.59819 HOMO: -7.40966 LUMO: 0.18232 factor:1 | 1 (-0.48017) | 1 | 1 |
| G: -6322.75232 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.76663 HOMO: -6.34570 LUMO: 0.41089 factor:1 | 1 (-0.64861) | -1 | -1 |
| G: -6322.75232 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.47653 HOMO: -6.78924 LUMO: 0.49525 factor:1 | 1 (-0.35851) | -1 | -1 |
| G: -6322.75232 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.49057 HOMO: -6.87632 LUMO: 0.44082 factor:1 | 1 (-0.37255) | -1 | -1 |
| G: -6322.75232 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.34504 HOMO: -6.69944 LUMO: 1.20546 factor:1 | 1 (-0.22702) | -1 | -1 |
| G: -6322.75232 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.61500 HOMO: -6.83006 LUMO: 1.28982 factor:1 | 1 (-0.49699) | -1 | -1 |
| G: -6322.75232 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.33919 HOMO: -7.78246 LUMO: 0.20681 factor:1 | 1 (-0.22117) | 1 | 1 |
| G: -6322.75232 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.33650 HOMO: -6.55794 LUMO: -1.65173 factor:1 | 1 (-0.21848) | -1 | -1 |
| G: -6322.75232 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.19353 HOMO: -6.77564 LUMO: -1.14560 factor:1 | 1 (-0.07551) | -1 | -1 |
| G: -6322.75232 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.33541 HOMO: -7.46680 LUMO: -1.18097 factor:1 | 1 (-0.21739) | 1 | 1 |
| G: -6322.75232 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.20477 HOMO: -6.88176 LUMO: -1.24900 factor:1 | 1 (-0.08675) | -1 | -1 |
| G: -6322.75232 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12586.96528 HOMO: -7.28177 LUMO: -0.42178 factor:1 | -1 (0.15274) | 1 | 1 |
| G: -6322.75232 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.44295 HOMO: -7.71715 LUMO: 0.19592 factor:1 | 1 (-0.32493) | 1 | 1 |
| G: -6322.75232 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.64031 HOMO: -7.02326 LUMO: -1.40683 factor:1 | 1 (-0.52230) | -1 | -1 |
| G: -6322.75232 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.83196 HOMO: -7.27088 LUMO: -1.07485 factor:1 | 1 (-0.71395) | 1 | 1 |
| G: -6322.75232 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.81838 HOMO: -7.17020 LUMO: -0.49525 factor:1 | 1 (-0.70037) | 1 | 1 |
| G: -6322.75232 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.61079 HOMO: -7.15932 LUMO: 0.02721 factor:1 | 1 (-0.49277) | 1 | 1 |
| G: -6322.75232 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.80676 HOMO: -7.00693 LUMO: -0.83267 factor:1 | 1 (-0.68875) | -1 | -1 |
| G: -6322.75232 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.81397 HOMO: -6.86543 LUMO: -0.10340 factor:1 | 1 (-0.69596) | -1 | -1 |
| G: -6322.75232 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.91980 HOMO: -7.11850 LUMO: -0.08980 factor:1 | 1 (-0.80178) | 1 | 1 |
| G: -6322.75232 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.69683 HOMO: -6.87087 LUMO: -0.88981 factor:1 | 1 (-0.57881) | -1 | -1 |
| G: -6322.75232 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.61838 HOMO: -7.08857 LUMO: -1.27077 factor:1 | 1 (-0.50036) | 1 | 1 |
| G: -6322.75232 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.60265 HOMO: -6.79468 LUMO: -0.81906 factor:1 | 1 (-0.48463) | -1 | -1 |
| G: -6322.75232 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.46610 HOMO: -6.86815 LUMO: -0.89798 factor:1 | 1 (-0.34809) | -1 | -1 |
| G: -6322.75232 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.39862 HOMO: -6.78652 LUMO: -2.00548 factor:1 | 1 (-0.28060) | -1 | -1 |
| G: -6322.75232 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.45351 HOMO: -6.75114 LUMO: -0.08436 factor:1 | 1 (-0.33549) | -1 | -1 |
| G: -6322.75232 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.47688 HOMO: -6.55794 LUMO: 0.52790 factor:1 | 1 (-0.35886) | -1 | -1 |
| G: -6322.75232 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.38599 HOMO: -7.17836 LUMO: 0.28300 factor:1 | 1 (-0.26798) | 1 | -1 |
| G: -6322.75232 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.67033 HOMO: -7.35796 LUMO: -0.77552 factor:1 | 1 (-0.55231) | 1 | 1 |
| G: -6322.75232 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.66442 HOMO: -7.23551 LUMO: -1.17553 factor:1 | 1 (-0.54640) | 1 | 1 |
| G: -6322.75232 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.67767 HOMO: -7.07496 LUMO: -1.14288 factor:1 | 1 (-0.55966) | 1 | 1 |
| G: -6322.75232 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.59743 HOMO: -6.70489 LUMO: -0.83539 factor:1 | 1 (-0.47941) | -1 | -1 |
| G: -6322.75232 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.35639 HOMO: -6.59604 LUMO: -0.89798 factor:1 | 1 (-0.23837) | -1 | -1 |
| G: -6322.75232 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.45541 HOMO: -6.94162 LUMO: -1.22451 factor:1 | 1 (-0.33739) | -1 | -1 |
| G: -6322.75232 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.39625 HOMO: -6.68040 LUMO: 0.22041 factor:1 | 1 (-0.27824) | -1 | -1 |
| G: -6322.75232 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.25522 HOMO: -6.88176 LUMO: 0.11157 factor:1 | 1 (-0.13720) | -1 | -1 |
| G: -6322.75232 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.51952 HOMO: -6.91713 LUMO: 1.27621 factor:1 | 1 (-0.40150) | -1 | -1 |
| G: -6322.75232 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.83389 HOMO: -6.77836 LUMO: 1.01226 factor:1 | 1 (-0.71588) | -1 | -1 |
| G: -6322.75232 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.53892 HOMO: -7.14571 LUMO: 1.48574 factor:1 | 1 (-0.42091) | 1 | 1 |
| G: -6322.75232 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.59070 HOMO: -6.96884 LUMO: 1.48574 factor:1 | 1 (-0.47269) | -1 | -1 |
| G: -6322.75232 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.66608 HOMO: -7.24367 LUMO: 1.28438 factor:1 | 1 (-0.54806) | 1 | 1 |
| G: -6322.75232 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.74687 HOMO: -7.10489 LUMO: 1.29526 factor:1 | 1 (-0.62886) | 1 | 1 |
| G: -6322.75232 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.70246 HOMO: -7.07224 LUMO: 1.29254 factor:1 | 1 (-0.58445) | 1 | 1 |
| G: -6322.75232 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.38719 HOMO: -7.12938 LUMO: 0.49253 factor:1 | 1 (-0.26918) | 1 | 1 |
| G: -6322.75232 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.54673 HOMO: -7.33619 LUMO: 1.45581 factor:1 | 1 (-0.42872) | 1 | 1 |
| G: -6322.75232 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.38009 HOMO: -6.87904 LUMO: -0.14422 factor:1 | 1 (-0.26207) | -1 | -1 |
| G: -6322.75232 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.74995 HOMO: -6.81917 LUMO: 0.50341 factor:1 | 1 (-0.63193) | -1 | -1 |
| G: -6322.75232 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.69033 HOMO: -7.27905 LUMO: 0.13606 factor:1 | 1 (-0.57231) | 1 | -1 |
| G: -6322.75232 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.63841 HOMO: -6.87904 LUMO: -0.09796 factor:1 | 1 (-0.52039) | -1 | -1 |
| G: -6322.75232 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.36512 HOMO: -7.33891 LUMO: 0.03810 factor:1 | 1 (-0.24711) | 1 | 1 |
| G: -6322.75232 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.43827 HOMO: -6.98516 LUMO: 0.98233 factor:1 | 1 (-0.32025) | -1 | -1 |
| G: -6322.75232 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.30986 HOMO: -6.94162 LUMO: 0.86804 factor:1 | 1 (-0.19184) | -1 | -1 |
| G: -6322.75232 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.19628 HOMO: -7.37701 LUMO: 0.05442 factor:1 | 1 (-0.07826) | 1 | 1 |
| G: -6322.75232 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12586.98457 HOMO: -7.04775 LUMO: 0.43266 factor:1 | -1 (0.13344) | -1 | -1 |
| G: -6322.75232 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.52787 HOMO: -7.47497 LUMO: 0.31837 factor:1 | 1 (-0.40986) | 1 | 1 |
| G: -6322.75232 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.40319 HOMO: -6.62053 LUMO: 0.13061 factor:1 | 1 (-0.28518) | -1 | -1 |
| G: -6322.45466 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12588.02195 HOMO: -6.44366 LUMO: -0.04354 factor:1 | 1 (-1.20160) | -1 | -1 |
| G: -6322.45466 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12588.08797 HOMO: -6.40284 LUMO: 0.68301 factor:1 | 1 (-1.26762) | -1 | -1 |
| G: -6322.45466 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12588.15719 HOMO: -6.73754 LUMO: 0.36735 factor:1 | 1 (-1.33684) | -1 | -1 |
| G: -6322.45466 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.78918 HOMO: -6.85455 LUMO: 0.23946 factor:1 | 1 (-0.96883) | -1 | -1 |
| G: -6322.45466 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.85993 HOMO: -6.93346 LUMO: 0.24762 factor:1 | 1 (-1.03958) | -1 | -1 |
| G: -6322.45466 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.69441 HOMO: -6.85455 LUMO: 0.17687 factor:1 | 1 (-0.87406) | -1 | -1 |
| G: -6322.45466 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12588.07695 HOMO: -6.62325 LUMO: 0.69933 factor:1 | 1 (-1.25659) | -1 | -1 |
| G: -6322.45466 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12588.08105 HOMO: -6.43005 LUMO: 0.50069 factor:1 | 1 (-1.26070) | -1 | -1 |
| G: -6322.45466 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.76791 HOMO: -6.56883 LUMO: 0.22858 factor:1 | 1 (-0.94755) | -1 | -1 |
| G: -6322.45466 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.67101 HOMO: -6.78380 LUMO: 0.54967 factor:1 | 1 (-0.85066) | -1 | -1 |
| G: -6322.45466 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.88989 HOMO: -7.35524 LUMO: 0.00272 factor:1 | 1 (-1.06954) | 1 | 1 |
| G: -6322.45466 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.50722 HOMO: -7.27360 LUMO: 0.08436 factor:1 | 1 (-0.68687) | 1 | 1 |
| G: -6322.45466 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.67724 HOMO: -7.44504 LUMO: -0.96056 factor:1 | 1 (-0.85689) | 1 | 1 |
| G: -6322.45466 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.71941 HOMO: -7.27360 LUMO: 0.29933 factor:1 | 1 (-0.89906) | 1 | 1 |
| G: -6322.45466 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.84644 HOMO: -7.09129 LUMO: 0.41089 factor:1 | 1 (-1.02609) | 1 | 1 |
| G: -6322.45466 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.95455 HOMO: -6.93618 LUMO: 0.36463 factor:1 | 1 (-1.13420) | -1 | -1 |
| G: -6322.45466 HOMO: -7.26000 LUMO: -3.02863 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.61090 HOMO: -7.65728 LUMO: 0.20136 factor:1 | 1 (-0.79055) | 1 | 1 |
| G: -6322.45466 HOMO: -7.26000 LUMO: -3.02863 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.66499 HOMO: -6.90353 LUMO: -0.92791 factor:1 | 1 (-0.84464) | -1 | -1 |
| G: -6322.45466 HOMO: -7.26000 LUMO: -3.02863 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.86538 HOMO: -6.82462 LUMO: -1.18370 factor:1 | 1 (-1.04503) | -1 | -1 |
| G: -6322.45466 HOMO: -7.26000 LUMO: -3.02863 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.86747 HOMO: -7.09129 LUMO: -0.13334 factor:1 | 1 (-1.04712) | 1 | 1 |
| G: -6322.45466 HOMO: -7.26000 LUMO: -3.02863 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.76527 HOMO: -7.40966 LUMO: -1.06941 factor:1 | 1 (-0.94492) | 1 | 1 |
| G: -6322.45466 HOMO: -7.26000 LUMO: -3.02863 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12588.05330 HOMO: -7.24367 LUMO: -1.00954 factor:1 | 1 (-1.23295) | 1 | 1 |
| G: -6322.45466 HOMO: -7.26000 LUMO: -3.02863 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.67560 HOMO: -7.51851 LUMO: 0.09796 factor:1 | 1 (-0.85525) | 1 | 1 |
| G: -6322.45466 HOMO: -7.26000 LUMO: -3.02863 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.47318 HOMO: -7.48857 LUMO: -0.07619 factor:1 | 1 (-0.65283) | 1 | 1 |
| G: -6322.45466 HOMO: -7.26000 LUMO: -3.02863 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.61928 HOMO: -6.53345 LUMO: 1.09390 factor:1 | 1 (-0.79893) | -1 | -1 |
| G: -6322.45466 HOMO: -7.26000 LUMO: -3.02863 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.67305 HOMO: -7.21918 LUMO: 0.08436 factor:1 | 1 (-0.85270) | 1 | 1 |
| G: -6322.45466 HOMO: -7.26000 LUMO: -3.02863 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.66535 HOMO: -7.38789 LUMO: 1.02587 factor:1 | 1 (-0.84500) | 1 | -1 |
| G: -6322.45466 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.56717 HOMO: -6.83550 LUMO: -0.67484 factor:1 | 1 (-0.74682) | -1 | -1 |
| G: -6322.45466 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.44978 HOMO: -7.04231 LUMO: 0.54151 factor:1 | 1 (-0.62943) | -1 | -1 |
| G: -6322.45466 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.25987 HOMO: -6.79740 LUMO: 1.91296 factor:1 | 1 (-0.43952) | 1 | 1 |
| G: -6322.45466 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.42795 HOMO: -7.35796 LUMO: -1.04220 factor:1 | 1 (-0.60760) | -1 | -1 |
| G: -6322.45466 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12588.04734 HOMO: -6.62597 LUMO: -0.44082 factor:1 | 1 (-1.22699) | -1 | -1 |
| G: -6322.45466 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.75074 HOMO: -6.45182 LUMO: -0.20409 factor:1 | 1 (-0.93038) | -1 | -1 |
| G: -6322.45466 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.73574 HOMO: -6.51168 LUMO: -0.23130 factor:1 | 1 (-0.91539) | -1 | -1 |
| G: -6322.45466 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.98834 HOMO: -7.14027 LUMO: 0.49797 factor:1 | 1 (-1.16799) | -1 | -1 |
| G: -6322.45466 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.66102 HOMO: -7.55660 LUMO: 0.24762 factor:1 | 1 (-0.84067) | -1 | -1 |
| G: -6322.45466 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.83457 HOMO: -6.88992 LUMO: -0.64763 factor:1 | 1 (-1.01422) | -1 | -1 |
| G: -6322.45466 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.92976 HOMO: -6.72665 LUMO: -0.45987 factor:1 | 1 (-1.10941) | -1 | -1 |
| G: -6322.45466 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.78118 HOMO: -6.72121 LUMO: -0.58232 factor:1 | 1 (-0.96083) | -1 | -1 |
| G: -6322.45466 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.50357 HOMO: -7.26816 LUMO: 0.32926 factor:1 | 1 (-0.68322) | -1 | -1 |
| G: -6322.45466 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.41321 HOMO: -6.57155 LUMO: -0.53606 factor:1 | 1 (-0.59285) | -1 | -1 |
| G: -6322.45466 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.73063 HOMO: -6.50896 LUMO: -0.43810 factor:1 | 1 (-0.91028) | -1 | -1 |
| G: -6322.45466 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.59851 HOMO: -6.73210 LUMO: -0.51430 factor:1 | 1 (-0.77816) | -1 | -1 |
| G: -6322.45466 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.74622 HOMO: -6.77019 LUMO: -0.62858 factor:1 | 1 (-0.92587) | -1 | -1 |
| G: -6322.45466 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.70526 HOMO: -6.82462 LUMO: -0.67484 factor:1 | 1 (-0.88491) | -1 | -1 |
| G: -6322.45466 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.59541 HOMO: -6.79740 LUMO: -0.55511 factor:1 | 1 (-0.77506) | -1 | -1 |
| G: -6322.45466 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.94924 HOMO: -6.79740 LUMO: -0.67756 factor:1 | 1 (-1.12889) | -1 | -1 |
| G: -6322.45466 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.73642 HOMO: -6.75114 LUMO: -0.55239 factor:1 | 1 (-0.91607) | -1 | -1 |
| G: -6322.45466 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.66611 HOMO: -6.49536 LUMO: -0.25307 factor:1 | 1 (-0.84576) | -1 | -1 |
| G: -6322.45466 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.60837 HOMO: -6.48992 LUMO: -0.25034 factor:1 | 1 (-0.78801) | -1 | -1 |
| G: -6322.45466 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.43944 HOMO: -6.52801 LUMO: -0.28028 factor:1 | 1 (-0.61909) | -1 | -1 |
| G: -6322.45466 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.51274 HOMO: -7.22462 LUMO: 0.52518 factor:1 | 1 (-0.69239) | -1 | -1 |
| G: -6322.45466 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.68897 HOMO: -6.59332 LUMO: -0.27211 factor:1 | 1 (-0.86861) | -1 | -1 |
| G: -6322.45466 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.72317 HOMO: -6.57427 LUMO: -0.16871 factor:1 | 1 (-0.90282) | -1 | -1 |
| G: -6322.45466 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.83591 HOMO: -6.71033 LUMO: 1.59187 factor:1 | 1 (-1.01556) | 1 | 1 |
| G: -6322.45466 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.56306 HOMO: -6.72121 LUMO: 2.00004 factor:1 | 1 (-0.74271) | 1 | 1 |
| G: -6322.45466 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.43650 HOMO: -6.61509 LUMO: 1.55921 factor:1 | 1 (-0.61615) | -1 | -1 |
| G: -6322.45466 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.40510 HOMO: -6.55250 LUMO: 1.73064 factor:1 | 1 (-0.58475) | -1 | -1 |
| G: -6322.45466 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.20942 HOMO: -6.66135 LUMO: 2.02181 factor:1 | 1 (-0.38907) | 1 | 1 |
| G: -6322.45466 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.86867 HOMO: -6.84911 LUMO: 1.98099 factor:1 | 1 (-1.04832) | 1 | 1 |
| G: -6322.45466 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.75710 HOMO: -6.66679 LUMO: 1.98371 factor:1 | 1 (-0.93675) | 1 | 1 |
| G: -6322.45466 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.63536 HOMO: -6.67495 LUMO: 2.04085 factor:1 | 1 (-0.81501) | 1 | 1 |
| G: -6322.45466 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.64581 HOMO: -6.89809 LUMO: 1.95106 factor:1 | 1 (-0.82546) | 1 | 1 |
| G: -6322.45466 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.80742 HOMO: -6.50352 LUMO: 1.88847 factor:1 | 1 (-0.98707) | -1 | -1 |
| G: -6322.45466 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.69180 HOMO: -6.93618 LUMO: 2.00004 factor:1 | 1 (-0.87144) | 1 | 1 |
| G: -6322.45466 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.89811 HOMO: -6.50896 LUMO: 1.73609 factor:1 | 1 (-1.07776) | -1 | -1 |
| G: -6322.45466 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.84276 HOMO: -6.69672 LUMO: 2.37283 factor:1 | 1 (-1.02241) | 1 | 1 |
| G: -6322.45466 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.61158 HOMO: -6.65591 LUMO: 2.20684 factor:1 | 1 (-0.79123) | 1 | 1 |
| G: -6322.45466 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.52845 HOMO: -6.23957 LUMO: 1.78507 factor:1 | 1 (-0.70809) | -1 | -1 |
| G: -6322.45466 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.53468 HOMO: -6.35114 LUMO: 1.92112 factor:1 | 1 (-0.71433) | -1 | -1 |
| G: -6322.45466 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.42469 HOMO: -6.53617 LUMO: 1.75241 factor:1 | 1 (-0.60434) | -1 | -1 |
| G: -6322.45466 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.94908 HOMO: -6.60420 LUMO: 1.78779 factor:1 | 1 (-1.12873) | 1 | 1 |
| G: -6322.45466 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.71463 HOMO: -7.40422 LUMO: -0.97145 factor:1 | 1 (-0.89427) | -1 | -1 |
| G: -6322.45466 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.59819 HOMO: -6.80013 LUMO: -0.69117 factor:1 | 1 (-0.77784) | -1 | -1 |
| G: -6322.45466 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.76663 HOMO: -6.68040 LUMO: -0.47076 factor:1 | 1 (-0.94628) | -1 | -1 |
| G: -6322.45466 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.47653 HOMO: -7.20285 LUMO: -0.66124 factor:1 | 1 (-0.65618) | -1 | -1 |
| G: -6322.45466 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.49057 HOMO: -6.82734 LUMO: -0.60137 factor:1 | 1 (-0.67022) | -1 | -1 |
| G: -6322.45466 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.34504 HOMO: -7.18653 LUMO: 0.59321 factor:1 | 1 (-0.52469) | -1 | -1 |
| G: -6322.45466 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.61500 HOMO: -7.29265 LUMO: 0.48164 factor:1 | 1 (-0.79465) | -1 | -1 |
| G: -6322.45466 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.33919 HOMO: -6.63414 LUMO: -0.25034 factor:1 | 1 (-0.51884) | -1 | -1 |
| G: -6322.45466 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.33650 HOMO: -7.20285 LUMO: 0.53879 factor:1 | 1 (-0.51615) | -1 | -1 |
| G: -6322.45466 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.19353 HOMO: -6.46815 LUMO: -0.21769 factor:1 | 1 (-0.37318) | -1 | -1 |
| G: -6322.45466 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.33541 HOMO: -6.57971 LUMO: -0.18776 factor:1 | 1 (-0.51506) | -1 | -1 |
| G: -6322.45466 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.20477 HOMO: -6.90897 LUMO: 1.91296 factor:1 | 1 (-0.38442) | 1 | 1 |
| G: -6322.45466 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12586.96528 HOMO: -6.67495 LUMO: 2.04358 factor:1 | 1 (-0.14493) | 1 | 1 |
| G: -6322.45466 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.44295 HOMO: -6.94162 LUMO: 1.73881 factor:1 | 1 (-0.62260) | 1 | 1 |
| G: -6322.45466 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.64031 HOMO: -6.73482 LUMO: 1.95922 factor:1 | 1 (-0.81996) | 1 | 1 |
| G: -6322.45466 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.83196 HOMO: -6.70489 LUMO: 2.04358 factor:1 | 1 (-1.01161) | 1 | 1 |
| G: -6322.45466 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.81838 HOMO: -7.04231 LUMO: 1.79323 factor:1 | 1 (-0.99803) | 1 | 1 |
| G: -6322.45466 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.61079 HOMO: -6.68584 LUMO: 1.60275 factor:1 | 1 (-0.79044) | 1 | 1 |
| G: -6322.45466 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.80676 HOMO: -6.40556 LUMO: 1.45581 factor:1 | 1 (-0.98641) | -1 | -1 |
| G: -6322.45466 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.81397 HOMO: -6.94979 LUMO: 2.16603 factor:1 | 1 (-0.99362) | 1 | 1 |
| G: -6322.45466 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.91980 HOMO: -6.84911 LUMO: 1.89935 factor:1 | 1 (-1.09945) | 1 | 1 |
| G: -6322.45466 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.69683 HOMO: -6.22052 LUMO: 1.57282 factor:1 | 1 (-0.87648) | -1 | -1 |
| G: -6322.45466 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.61838 HOMO: -6.51168 LUMO: 2.10072 factor:1 | 1 (-0.79803) | -1 | -1 |
| G: -6322.45466 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.60265 HOMO: -7.03686 LUMO: 2.12249 factor:1 | 1 (-0.78230) | 1 | 1 |
| G: -6322.45466 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.46610 HOMO: -6.84094 LUMO: 1.63268 factor:1 | 1 (-0.64575) | 1 | 1 |
| G: -6322.45466 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.39862 HOMO: -6.75387 LUMO: 1.72248 factor:1 | 1 (-0.57827) | 1 | 1 |
| G: -6322.45466 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.45351 HOMO: -6.86271 LUMO: 1.68711 factor:1 | 1 (-0.63315) | 1 | 1 |
| G: -6322.45466 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.47688 HOMO: -6.84094 LUMO: 2.02997 factor:1 | 1 (-0.65653) | 1 | 1 |
| G: -6322.45466 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.38599 HOMO: -6.80557 LUMO: 2.02725 factor:1 | 1 (-0.56564) | 1 | 1 |
| G: -6322.45466 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.67033 HOMO: -6.38651 LUMO: 1.53472 factor:1 | 1 (-0.84997) | -1 | -1 |
| G: -6322.45466 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.66442 HOMO: -7.51306 LUMO: 0.28572 factor:1 | 1 (-0.84407) | -1 | -1 |
| G: -6322.45466 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.67767 HOMO: -6.97972 LUMO: -0.74287 factor:1 | 1 (-0.85732) | -1 | -1 |
| G: -6322.45466 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.59743 HOMO: -6.83822 LUMO: -0.65852 factor:1 | 1 (-0.77708) | -1 | -1 |
| G: -6322.45466 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.35639 HOMO: -6.71305 LUMO: -0.49525 factor:1 | 1 (-0.53604) | -1 | -1 |
| G: -6322.45466 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.45541 HOMO: -6.60692 LUMO: -0.22313 factor:1 | 1 (-0.63506) | -1 | -1 |
| G: -6322.45466 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.39625 HOMO: -7.20013 LUMO: 0.55239 factor:1 | 1 (-0.57590) | -1 | -1 |
| G: -6322.45466 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.25522 HOMO: -6.60420 LUMO: -0.28028 factor:1 | 1 (-0.43487) | -1 | -1 |
| G: -6322.45466 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.51952 HOMO: -6.69128 LUMO: -0.30477 factor:1 | 1 (-0.69917) | -1 | -1 |
| G: -6322.45466 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.83389 HOMO: -6.65591 LUMO: -0.25579 factor:1 | 1 (-1.01354) | -1 | -1 |
| G: -6322.45466 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.53892 HOMO: -6.69128 LUMO: 1.70888 factor:1 | 1 (-0.71857) | 1 | 1 |
| G: -6322.45466 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.59070 HOMO: -6.50080 LUMO: 1.87759 factor:1 | 1 (-0.77035) | -1 | -1 |
| G: -6322.45466 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.66608 HOMO: -6.85727 LUMO: 1.99187 factor:1 | 1 (-0.84573) | 1 | 1 |
| G: -6322.45466 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.74687 HOMO: -6.58788 LUMO: 1.79051 factor:1 | 1 (-0.92652) | 1 | 1 |
| G: -6322.45466 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.70246 HOMO: -6.64230 LUMO: 2.16058 factor:1 | 1 (-0.88211) | 1 | 1 |
| G: -6322.45466 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.38719 HOMO: -6.58788 LUMO: 2.10616 factor:1 | 1 (-0.56684) | 1 | 1 |
| G: -6322.45466 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.54673 HOMO: -7.01782 LUMO: 2.13609 factor:1 | 1 (-0.72638) | 1 | 1 |
| G: -6322.45466 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.38009 HOMO: -6.31304 LUMO: 2.31841 factor:1 | 1 (-0.55974) | -1 | -1 |
| G: -6322.45466 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.74995 HOMO: -6.94979 LUMO: 2.07895 factor:1 | 1 (-0.92960) | 1 | 1 |
| G: -6322.45466 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.69033 HOMO: -6.88992 LUMO: 2.28031 factor:1 | 1 (-0.86998) | 1 | 1 |
| G: -6322.45466 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.63841 HOMO: -6.66407 LUMO: 2.07623 factor:1 | 1 (-0.81806) | 1 | 1 |
| G: -6322.45466 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.36512 HOMO: -6.52529 LUMO: 1.70071 factor:1 | 1 (-0.54477) | -1 | -1 |
| G: -6322.45466 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.43827 HOMO: -6.58788 LUMO: 1.57282 factor:1 | 1 (-0.61792) | -1 | -1 |
| G: -6322.45466 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.30986 HOMO: -6.55250 LUMO: 1.95378 factor:1 | 1 (-0.48951) | -1 | -1 |
| G: -6322.45466 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.19628 HOMO: -6.24773 LUMO: 1.77962 factor:1 | 1 (-0.37593) | -1 | -1 |
| G: -6322.45466 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12586.98457 HOMO: -6.31304 LUMO: 2.18507 factor:1 | 1 (-0.16422) | -1 | -1 |
| G: -6322.45466 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.52787 HOMO: -6.18243 LUMO: 2.01636 factor:1 | 1 (-0.70752) | -1 | -1 |
| G: -6322.45466 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.40319 HOMO: -6.99877 LUMO: 2.14970 factor:1 | 1 (-0.58284) | 1 | 1 |
| G: -6322.66432 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12588.02195 HOMO: -6.72665 LUMO: 2.07079 factor:1 | 1 (-0.99194) | 1 | 1 |
| G: -6322.66432 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12588.08797 HOMO: -6.36202 LUMO: 2.17419 factor:1 | 1 (-1.05795) | -1 | -1 |
| G: -6322.66432 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12588.15719 HOMO: -6.78652 LUMO: 2.05718 factor:1 | 1 (-1.12718) | 1 | -1 |
| G: -6322.66432 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.78918 HOMO: -6.87360 LUMO: 2.34290 factor:1 | 1 (-0.75917) | 1 | 1 |
| G: -6322.66432 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.85993 HOMO: -6.62053 LUMO: 1.89391 factor:1 | 1 (-0.82992) | 1 | 1 |
| G: -6322.66432 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.69441 HOMO: -6.58788 LUMO: 1.83133 factor:1 | 1 (-0.66439) | 1 | 1 |
| G: -6322.66432 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12588.07695 HOMO: -7.08584 LUMO: 1.91568 factor:1 | 1 (-1.04693) | 1 | 1 |
| G: -6322.66432 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12588.08105 HOMO: -6.56883 LUMO: 1.81228 factor:1 | 1 (-1.05104) | 1 | 1 |
| G: -6322.66432 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.76791 HOMO: -6.66135 LUMO: 1.92384 factor:1 | 1 (-0.73789) | 1 | 1 |
| G: -6322.66432 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.67101 HOMO: -6.64502 LUMO: 2.15786 factor:1 | 1 (-0.64099) | 1 | 1 |
| G: -6322.66432 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.88989 HOMO: -6.71305 LUMO: 1.91840 factor:1 | 1 (-0.85988) | 1 | 1 |
| G: -6322.66432 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.50722 HOMO: -6.44094 LUMO: 1.74425 factor:1 | 1 (-0.47721) | -1 | -1 |
| G: -6322.66432 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.67724 HOMO: -6.51985 LUMO: 1.84221 factor:1 | 1 (-0.64722) | -1 | -1 |
| G: -6322.66432 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.71941 HOMO: -6.63414 LUMO: -0.24762 factor:1 | 1 (-0.68940) | -1 | -1 |
| G: -6322.66432 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.84644 HOMO: -6.60420 LUMO: -0.22585 factor:1 | 1 (-0.81642) | -1 | -1 |
| G: -6322.66432 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.95455 HOMO: -7.19741 LUMO: 0.58232 factor:1 | 1 (-0.92453) | -1 | -1 |
| G: -6322.66432 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.61090 HOMO: -6.77019 LUMO: -0.56872 factor:1 | 1 (-0.58088) | -1 | -1 |
| G: -6322.66432 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.66499 HOMO: -7.46136 LUMO: 0.28844 factor:1 | 1 (-0.63498) | -1 | -1 |
| G: -6322.66432 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.86538 HOMO: -6.60420 LUMO: -0.54151 factor:1 | 1 (-0.83536) | -1 | -1 |
| G: -6322.66432 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.86747 HOMO: -6.53890 LUMO: -0.46531 factor:1 | 1 (-0.83746) | -1 | -1 |
| G: -6322.66432 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.76527 HOMO: -6.81645 LUMO: -0.57144 factor:1 | 1 (-0.73525) | -1 | -1 |
| G: -6322.66432 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12588.05330 HOMO: -7.48041 LUMO: 0.28572 factor:1 | 1 (-1.02328) | -1 | -1 |
| G: -6322.66432 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.67560 HOMO: -6.75659 LUMO: -0.45715 factor:1 | 1 (-0.64559) | -1 | -1 |
| G: -6322.66432 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.47318 HOMO: -6.66135 LUMO: -0.41906 factor:1 | 1 (-0.44316) | -1 | -1 |
| G: -6322.66432 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.61928 HOMO: -6.55794 LUMO: -0.27483 factor:1 | 1 (-0.58926) | -1 | -1 |
| G: -6322.66432 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.67305 HOMO: -7.07496 LUMO: -0.63403 factor:1 | 1 (-0.64303) | -1 | -1 |
| G: -6322.66432 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.66535 HOMO: -7.12394 LUMO: 0.53334 factor:1 | 1 (-0.63533) | -1 | -1 |
| G: -6322.66432 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.56717 HOMO: -6.53617 LUMO: -0.25579 factor:1 | 1 (-0.53715) | -1 | -1 |
| G: -6322.66432 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.44978 HOMO: -6.50896 LUMO: -0.25034 factor:1 | 1 (-0.41976) | -1 | -1 |
| G: -6322.66432 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.25987 HOMO: -7.17564 LUMO: -0.68573 factor:1 | 1 (-0.22985) | -1 | -1 |
| G: -6322.66432 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.42795 HOMO: -6.53617 LUMO: -0.30749 factor:1 | 1 (-0.39794) | -1 | -1 |
| G: -6322.66432 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12588.04734 HOMO: -6.55522 LUMO: -0.30749 factor:1 | 1 (-1.01732) | -1 | -1 |
| G: -6322.66432 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.75074 HOMO: -7.05591 LUMO: -0.71022 factor:1 | 1 (-0.72072) | -1 | -1 |
| G: -6322.66432 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.73574 HOMO: -7.17564 LUMO: -0.69933 factor:1 | 1 (-0.70573) | -1 | -1 |
| G: -6322.66432 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.98834 HOMO: -6.78380 LUMO: -0.67756 factor:1 | 1 (-0.95833) | -1 | -1 |
| G: -6322.66432 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.66102 HOMO: -6.62325 LUMO: 2.02725 factor:1 | 1 (-0.63100) | 1 | 1 |
| G: -6322.66432 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.83457 HOMO: -6.63414 LUMO: 1.91296 factor:1 | 1 (-0.80456) | 1 | -1 |
| G: -6322.66432 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.92976 HOMO: -6.83278 LUMO: 1.65717 factor:1 | 1 (-0.89974) | 1 | 1 |
| G: -6322.66432 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.78118 HOMO: -6.66407 LUMO: 1.95650 factor:1 | 1 (-0.75117) | 1 | 1 |
| G: -6322.66432 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.50357 HOMO: -6.61237 LUMO: 2.11432 factor:1 | 1 (-0.47356) | 1 | 1 |
| G: -6322.66432 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.41321 HOMO: -6.62053 LUMO: 2.09256 factor:1 | 1 (-0.38319) | 1 | -1 |
| G: -6322.66432 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.73063 HOMO: -6.78652 LUMO: 2.13609 factor:1 | 1 (-0.70061) | 1 | 1 |
| G: -6322.66432 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.59851 HOMO: -6.94707 LUMO: 1.81772 factor:1 | 1 (-0.56850) | 1 | 1 |
| G: -6322.66432 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.74622 HOMO: -6.85183 LUMO: 2.12793 factor:1 | 1 (-0.71620) | 1 | 1 |
| G: -6322.66432 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.70526 HOMO: -6.81101 LUMO: 1.83949 factor:1 | 1 (-0.67525) | 1 | 1 |
| G: -6322.66432 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.59541 HOMO: -6.98788 LUMO: 2.16058 factor:1 | 1 (-0.56540) | 1 | 1 |
| G: -6322.66432 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.94924 HOMO: -6.62869 LUMO: 2.00820 factor:1 | 1 (-0.91923) | 1 | 1 |
| G: -6322.66432 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.73642 HOMO: -6.34025 LUMO: 2.25855 factor:1 | 1 (-0.70641) | -1 | -1 |
| G: -6322.66432 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.66611 HOMO: -6.01372 LUMO: 2.01636 factor:1 | 1 (-0.63609) | -1 | -1 |
| G: -6322.66432 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.60837 HOMO: -6.89264 LUMO: 2.27487 factor:1 | 1 (-0.57835) | 1 | 1 |
| G: -6322.66432 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.43944 HOMO: -6.53073 LUMO: 2.20684 factor:1 | 1 (-0.40942) | -1 | -1 |
| G: -6322.66432 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.51274 HOMO: -6.83278 LUMO: 1.53744 factor:1 | 1 (-0.48273) | -1 | -1 |
| G: -6322.66432 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.68897 HOMO: -6.41917 LUMO: 1.82316 factor:1 | 1 (-0.65895) | -1 | -1 |
| G: -6322.66432 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.72317 HOMO: -6.56339 LUMO: 1.63813 factor:1 | 1 (-0.69316) | -1 | -1 |
| G: -6322.66432 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.83591 HOMO: -6.88992 LUMO: 1.65173 factor:1 | 1 (-0.80589) | 1 | 1 |
| G: -6322.66432 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.56306 HOMO: -6.63141 LUMO: 1.92112 factor:1 | 1 (-0.53304) | 1 | 1 |
| G: -6322.66432 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.43650 HOMO: -6.83822 LUMO: 1.88847 factor:1 | 1 (-0.40648) | 1 | 1 |
| G: -6322.66432 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.40510 HOMO: -6.84638 LUMO: 1.90480 factor:1 | 1 (-0.37508) | 1 | 1 |
| G: -6322.66432 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.20942 HOMO: -6.82462 LUMO: 1.70888 factor:1 | 1 (-0.17940) | 1 | 1 |
| G: -6322.66432 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.86867 HOMO: -6.82734 LUMO: 2.12521 factor:1 | 1 (-0.83865) | 1 | 1 |
| G: -6322.66432 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.75710 HOMO: -6.94435 LUMO: 1.87214 factor:1 | 1 (-0.72709) | 1 | 1 |
| G: -6322.66432 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.63536 HOMO: -6.98516 LUMO: 2.51433 factor:1 | 1 (-0.60534) | 1 | 1 |
| G: -6322.66432 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.64581 HOMO: -6.74026 LUMO: 2.15514 factor:1 | 1 (-0.61579) | 1 | 1 |
| G: -6322.66432 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.80742 HOMO: -6.93618 LUMO: 2.54426 factor:1 | 1 (-0.77740) | 1 | 1 |
| G: -6322.66432 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.69180 HOMO: -6.28583 LUMO: 2.53610 factor:1 | 1 (-0.66178) | -1 | -1 |
| G: -6322.66432 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.89811 HOMO: -6.56883 LUMO: 1.94834 factor:1 | 1 (-0.86810) | 1 | 1 |
| G: -6322.66432 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.84276 HOMO: -7.08584 LUMO: 1.99187 factor:1 | 1 (-0.81275) | 1 | 1 |
| G: -6322.66432 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.61158 HOMO: -6.19059 LUMO: 1.99732 factor:1 | 1 (-0.58156) | -1 | -1 |
| G: -6322.66432 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.52845 HOMO: -6.78108 LUMO: 2.03813 factor:1 | 1 (-0.49843) | 1 | 1 |
| G: -6322.66432 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.53468 HOMO: -6.82189 LUMO: 1.77418 factor:1 | 1 (-0.50466) | 1 | 1 |
| G: -6322.66432 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.42469 HOMO: -6.45454 LUMO: 1.78779 factor:1 | 1 (-0.39467) | -1 | -1 |
| G: -6322.66432 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.94908 HOMO: -6.84366 LUMO: 1.77690 factor:1 | 1 (-0.91906) | 1 | 1 |
| G: -6322.66432 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.71463 HOMO: -6.74026 LUMO: 1.67622 factor:1 | 1 (-0.68461) | 1 | 1 |
| G: -6322.66432 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.59819 HOMO: -6.76475 LUMO: 2.40277 factor:1 | 1 (-0.56817) | 1 | 1 |
| G: -6322.66432 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.76663 HOMO: -6.65863 LUMO: 1.86670 factor:1 | 1 (-0.73661) | 1 | 1 |
| G: -6322.66432 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.47653 HOMO: -6.50080 LUMO: 1.93201 factor:1 | 1 (-0.44651) | -1 | -1 |
| G: -6322.66432 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.49057 HOMO: -6.34842 LUMO: 1.70888 factor:1 | 1 (-0.46055) | -1 | -1 |
| G: -6322.66432 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.34504 HOMO: -6.60692 LUMO: 2.20140 factor:1 | 1 (-0.31503) | 1 | 1 |
| G: -6322.66432 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.61500 HOMO: -6.74026 LUMO: 2.14970 factor:1 | 1 (-0.58499) | 1 | 1 |
| G: -6322.66432 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.33919 HOMO: -6.63686 LUMO: 2.17419 factor:1 | 1 (-0.30918) | 1 | 1 |
| G: -6322.66432 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.33650 HOMO: -6.81917 LUMO: 2.10072 factor:1 | 1 (-0.30648) | 1 | -1 |
| G: -6322.66432 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.19353 HOMO: -6.92802 LUMO: 2.04358 factor:1 | 1 (-0.16351) | 1 | 1 |
| G: -6322.66432 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.33541 HOMO: -6.56067 LUMO: -0.47620 factor:1 | 1 (-0.30539) | -1 | -1 |
| G: -6322.66432 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.20477 HOMO: -6.56611 LUMO: -0.77008 factor:1 | 1 (-0.17475) | -1 | -1 |
| G: -6322.66432 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12586.96528 HOMO: -6.78380 LUMO: -0.64763 factor:1 | -1 (0.06474) | -1 | -1 |
| G: -6322.66432 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.44295 HOMO: -6.51985 LUMO: -0.24490 factor:1 | 1 (-0.41293) | -1 | -1 |
| G: -6322.66432 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.64031 HOMO: -6.52529 LUMO: -0.27483 factor:1 | 1 (-0.61030) | -1 | -1 |
| G: -6322.66432 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.83196 HOMO: -7.10489 LUMO: -0.62586 factor:1 | 1 (-0.80195) | -1 | -1 |
| G: -6322.66432 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.81838 HOMO: -7.18108 LUMO: 0.48980 factor:1 | 1 (-0.78837) | -1 | -1 |
| G: -6322.66432 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.61079 HOMO: -7.14299 LUMO: -0.63947 factor:1 | 1 (-0.58077) | -1 | -1 |
| G: -6322.66432 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.80676 HOMO: -6.70761 LUMO: -0.54423 factor:1 | 1 (-0.77675) | -1 | -1 |
| G: -6322.66432 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.81397 HOMO: -7.32258 LUMO: -1.03675 factor:1 | 1 (-0.78396) | -1 | -1 |
| G: -6322.66432 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.91980 HOMO: -6.65046 LUMO: -0.41361 factor:1 | 1 (-0.88979) | -1 | -1 |
| G: -6322.66432 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.69683 HOMO: -6.76475 LUMO: -0.60137 factor:1 | 1 (-0.66682) | -1 | -1 |
| G: -6322.66432 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.61838 HOMO: -6.77836 LUMO: -0.54423 factor:1 | 1 (-0.58836) | -1 | -1 |
| G: -6322.66432 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.60265 HOMO: -7.52395 LUMO: 0.26395 factor:1 | 1 (-0.57264) | -1 | -1 |
| G: -6322.66432 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.46610 HOMO: -6.93890 LUMO: -0.72382 factor:1 | 1 (-0.43609) | -1 | -1 |
| G: -6322.66432 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.39862 HOMO: -6.72938 LUMO: -0.47348 factor:1 | 1 (-0.36861) | -1 | -1 |
| G: -6322.66432 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.45351 HOMO: -6.66951 LUMO: -0.40817 factor:1 | 1 (-0.42349) | -1 | -1 |
| G: -6322.66432 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.47688 HOMO: -6.60420 LUMO: -0.19320 factor:1 | 1 (-0.44687) | -1 | -1 |
| G: -6322.66432 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.38599 HOMO: -6.67495 LUMO: -0.27211 factor:1 | 1 (-0.35598) | -1 | -1 |
| G: -6322.66432 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.67033 HOMO: -7.23823 LUMO: -0.62858 factor:1 | 1 (-0.64031) | -1 | -1 |
| G: -6322.66432 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.66442 HOMO: -7.27088 LUMO: 0.53334 factor:1 | 1 (-0.63441) | -1 | -1 |
| G: -6322.66432 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.67767 HOMO: -7.20013 LUMO: 0.59049 factor:1 | 1 (-0.64766) | -1 | -1 |
| G: -6322.66432 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.59743 HOMO: -6.60148 LUMO: -0.20953 factor:1 | 1 (-0.56741) | -1 | -1 |
| G: -6322.66432 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.35639 HOMO: -6.69400 LUMO: -0.51974 factor:1 | 1 (-0.32637) | -1 | -1 |
| G: -6322.66432 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.45541 HOMO: -7.40422 LUMO: -0.98777 factor:1 | 1 (-0.42540) | -1 | -1 |
| G: -6322.66432 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.39625 HOMO: -6.88176 LUMO: -0.71022 factor:1 | 1 (-0.36624) | -1 | -1 |
| G: -6322.66432 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.25522 HOMO: -6.86271 LUMO: -0.59321 factor:1 | 1 (-0.22520) | -1 | -1 |
| G: -6322.66432 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.51952 HOMO: -6.73754 LUMO: -0.55239 factor:1 | 1 (-0.48951) | -1 | -1 |
| G: -6322.66432 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.83389 HOMO: -6.71033 LUMO: 1.57010 factor:1 | 1 (-0.80388) | -1 | -1 |
| G: -6322.66432 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.53892 HOMO: -6.69672 LUMO: 1.68711 factor:1 | 1 (-0.50891) | 1 | 1 |
| G: -6322.66432 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.59070 HOMO: -6.67495 LUMO: 2.03813 factor:1 | 1 (-0.56069) | 1 | 1 |
| G: -6322.66432 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.66608 HOMO: -6.54434 LUMO: 1.83677 factor:1 | 1 (-0.63607) | -1 | -1 |
| G: -6322.66432 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.74687 HOMO: -6.57155 LUMO: 1.77146 factor:1 | 1 (-0.71686) | 1 | 1 |
| G: -6322.66432 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.70246 HOMO: -6.76747 LUMO: 1.87759 factor:1 | 1 (-0.67245) | 1 | 1 |
| G: -6322.66432 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.38719 HOMO: -6.58243 LUMO: 1.61364 factor:1 | 1 (-0.35718) | 1 | 1 |
| G: -6322.66432 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.54673 HOMO: -6.61781 LUMO: 2.13881 factor:1 | 1 (-0.51672) | 1 | 1 |
| G: -6322.66432 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.38009 HOMO: -6.62597 LUMO: 2.00276 factor:1 | 1 (-0.35007) | 1 | 1 |
| G: -6322.66432 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.74995 HOMO: -7.01237 LUMO: 1.95922 factor:1 | 1 (-0.71993) | 1 | 1 |
| G: -6322.66432 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.69033 HOMO: -7.03959 LUMO: 2.16875 factor:1 | 1 (-0.66031) | 1 | 1 |
| G: -6322.66432 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.63841 HOMO: -6.83278 LUMO: 1.91296 factor:1 | 1 (-0.60839) | 1 | 1 |
| G: -6322.66432 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.36512 HOMO: -6.40012 LUMO: 1.95650 factor:1 | 1 (-0.33511) | -1 | -1 |
| G: -6322.66432 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.43827 HOMO: -6.50080 LUMO: 1.73337 factor:1 | 1 (-0.40825) | -1 | -1 |
| G: -6322.66432 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.30986 HOMO: -6.95795 LUMO: 2.28848 factor:1 | 1 (-0.27984) | 1 | 1 |
| G: -6322.66432 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.19628 HOMO: -6.63686 LUMO: 2.20140 factor:1 | 1 (-0.16626) | 1 | -1 |
| G: -6322.66432 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12586.98457 HOMO: -6.57427 LUMO: 1.87214 factor:1 | -1 (0.04544) | 1 | -1 |
| G: -6322.66432 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.52787 HOMO: -6.38379 LUMO: 2.32113 factor:1 | 1 (-0.49786) | -1 | -1 |
| G: -6322.66432 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.40319 HOMO: -6.63958 LUMO: 2.04902 factor:1 | 1 (-0.37318) | 1 | 1 |
| G: -6323.39516 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12588.02195 HOMO: -6.70216 LUMO: 1.93201 factor:1 | 1 (-0.26109) | 1 | 1 |
| G: -6323.39516 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12588.08797 HOMO: -6.80557 LUMO: 2.23678 factor:1 | 1 (-0.32711) | 1 | 1 |
| G: -6323.39516 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12588.15719 HOMO: -6.72938 LUMO: 2.28304 factor:1 | 1 (-0.39633) | 1 | 1 |
| G: -6323.39516 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.78918 HOMO: -6.56067 LUMO: 1.66806 factor:1 | 1 (-0.02833) | -1 | -1 |
| G: -6323.39516 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.85993 HOMO: -6.95523 LUMO: 2.33474 factor:1 | 1 (-0.09908) | 1 | 1 |
| G: -6323.39516 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.69441 HOMO: -6.59876 LUMO: 2.30480 factor:1 | -1 (0.06645) | 1 | 1 |
| G: -6323.39516 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12588.07695 HOMO: -6.87360 LUMO: 1.75786 factor:1 | 1 (-0.31609) | 1 | 1 |
| G: -6323.39516 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12588.08105 HOMO: -7.06408 LUMO: 1.99187 factor:1 | 1 (-0.32020) | 1 | 1 |
| G: -6323.39516 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.76791 HOMO: -6.95795 LUMO: 1.88847 factor:1 | 1 (-0.00705) | 1 | 1 |
| G: -6323.39516 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.67101 HOMO: -6.85455 LUMO: 1.63813 factor:1 | -1 (0.08985) | 1 | 1 |
| G: -6323.39516 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.88989 HOMO: -7.09129 LUMO: 2.31569 factor:1 | 1 (-0.12904) | 1 | 1 |
| G: -6323.39516 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.50722 HOMO: -6.91441 LUMO: 1.68983 factor:1 | -1 (0.25364) | 1 | 1 |
| G: -6323.39516 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.67724 HOMO: -6.89809 LUMO: 2.23678 factor:1 | -1 (0.08362) | 1 | 1 |
| G: -6323.39516 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.71941 HOMO: -6.78652 LUMO: 1.98371 factor:1 | -1 (0.04144) | 1 | -1 |
| G: -6323.39516 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.84644 HOMO: -6.94707 LUMO: 2.23678 factor:1 | 1 (-0.08558) | 1 | 1 |
| G: -6323.39516 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.95455 HOMO: -7.07224 LUMO: 2.13337 factor:1 | 1 (-0.19369) | 1 | 1 |
| G: -6323.39516 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.61090 HOMO: -6.94979 LUMO: 2.28031 factor:1 | -1 (0.14996) | 1 | 1 |
| G: -6323.39516 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.66499 HOMO: -6.60965 LUMO: 2.20412 factor:1 | -1 (0.09587) | 1 | 1 |
| G: -6323.39516 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.86538 HOMO: -6.87360 LUMO: 2.40277 factor:1 | 1 (-0.10452) | 1 | -1 |
| G: -6323.39516 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.86747 HOMO: -6.92802 LUMO: 1.89663 factor:1 | 1 (-0.10661) | 1 | -1 |
| G: -6323.39516 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.76527 HOMO: -6.88448 LUMO: 2.02725 factor:1 | 1 (-0.00441) | 1 | 1 |
| G: -6323.39516 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12588.05330 HOMO: -6.69128 LUMO: 1.55105 factor:1 | 1 (-0.29244) | -1 | -1 |
| G: -6323.39516 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.67560 HOMO: -6.54978 LUMO: 1.93201 factor:1 | -1 (0.08525) | -1 | -1 |
| G: -6323.39516 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.47318 HOMO: -6.19331 LUMO: 1.46941 factor:1 | -1 (0.28768) | -1 | -1 |
| G: -6323.39516 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.61928 HOMO: -6.55794 LUMO: 1.89663 factor:1 | -1 (0.14158) | -1 | -1 |
| G: -6323.39516 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.67305 HOMO: -6.07630 LUMO: 1.94289 factor:1 | -1 (0.08781) | -1 | -1 |
| G: -6323.39516 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.66535 HOMO: -7.46408 LUMO: 0.31565 factor:1 | -1 (0.09551) | -1 | -1 |
| G: -6323.39516 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.56717 HOMO: -6.63958 LUMO: -0.61770 factor:1 | -1 (0.19369) | -1 | -1 |
| G: -6323.39516 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.44978 HOMO: -6.81101 LUMO: -0.57960 factor:1 | -1 (0.31108) | -1 | -1 |
| G: -6323.39516 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.25987 HOMO: -6.74298 LUMO: -0.57960 factor:1 | -1 (0.50099) | -1 | -1 |
| G: -6323.39516 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.42795 HOMO: -6.63686 LUMO: -0.42994 factor:1 | -1 (0.33290) | -1 | -1 |
| G: -6323.39516 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12588.04734 HOMO: -6.60965 LUMO: -0.41089 factor:1 | 1 (-0.28648) | -1 | -1 |
| G: -6323.39516 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.75074 HOMO: -6.60692 LUMO: -0.80274 factor:1 | -1 (0.01012) | -1 | -1 |
| G: -6323.39516 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.73574 HOMO: -6.58788 LUMO: -0.78097 factor:1 | -1 (0.02512) | -1 | -1 |
| G: -6323.39516 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.98834 HOMO: -6.67767 LUMO: -0.48436 factor:1 | 1 (-0.22749) | -1 | -1 |
| G: -6323.39516 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.66102 HOMO: -6.63141 LUMO: -0.40545 factor:1 | -1 (0.09984) | -1 | -1 |
| G: -6323.39516 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.83457 HOMO: -6.62053 LUMO: -0.83811 factor:1 | 1 (-0.07372) | -1 | -1 |
| G: -6323.39516 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.92976 HOMO: -6.59604 LUMO: -0.35375 factor:1 | 1 (-0.16890) | -1 | -1 |
| G: -6323.39516 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.78118 HOMO: -6.34297 LUMO: -0.39729 factor:1 | 1 (-0.02033) | -1 | -1 |
| G: -6323.39516 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.50357 HOMO: -6.67223 LUMO: 1.97827 factor:1 | -1 (0.25728) | 1 | 1 |
| G: -6323.39516 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.41321 HOMO: -6.40012 LUMO: 1.89935 factor:1 | -1 (0.34765) | -1 | -1 |
| G: -6323.39516 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.73063 HOMO: -6.74842 LUMO: 1.97283 factor:1 | -1 (0.03023) | 1 | -1 |
| G: -6323.39516 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.59851 HOMO: -6.76747 LUMO: 2.17147 factor:1 | -1 (0.16234) | 1 | 1 |
| G: -6323.39516 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.74622 HOMO: -6.72121 LUMO: 1.55649 factor:1 | -1 (0.01464) | -1 | -1 |
| G: -6323.39516 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.70526 HOMO: -6.97700 LUMO: 2.04085 factor:1 | -1 (0.05559) | 1 | 1 |
| G: -6323.39516 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.59541 HOMO: -7.06680 LUMO: 2.04085 factor:1 | -1 (0.16545) | 1 | -1 |
| G: -6323.39516 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.94924 HOMO: -7.09673 LUMO: 2.35106 factor:1 | 1 (-0.18838) | 1 | 1 |
| G: -6323.39516 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.73642 HOMO: -6.83006 LUMO: 2.14970 factor:1 | -1 (0.02444) | 1 | 1 |
| G: -6323.39516 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.66611 HOMO: -6.72665 LUMO: 2.20140 factor:1 | -1 (0.09475) | 1 | -1 |
| G: -6323.39516 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.60837 HOMO: -6.77291 LUMO: 2.34562 factor:1 | -1 (0.15249) | 1 | -1 |
| G: -6323.39516 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.43944 HOMO: -6.73754 LUMO: 2.00276 factor:1 | -1 (0.32142) | 1 | -1 |
| G: -6323.39516 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.51274 HOMO: -7.04231 LUMO: 1.92112 factor:1 | -1 (0.24811) | 1 | -1 |
| G: -6323.39516 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.68897 HOMO: -6.83822 LUMO: 1.72248 factor:1 | -1 (0.07189) | 1 | 1 |
| G: -6323.39516 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.72317 HOMO: -6.57971 LUMO: 2.16603 factor:1 | -1 (0.03769) | 1 | -1 |
| G: -6323.39516 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.83591 HOMO: -6.80013 LUMO: 1.88575 factor:1 | 1 (-0.07505) | 1 | 1 |
| G: -6323.39516 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.56306 HOMO: -6.93618 LUMO: 2.18235 factor:1 | -1 (0.19780) | 1 | 1 |
| G: -6323.39516 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.43650 HOMO: -6.54706 LUMO: 1.91024 factor:1 | -1 (0.32436) | -1 | -1 |
| G: -6323.39516 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.40510 HOMO: -7.06952 LUMO: 2.18507 factor:1 | -1 (0.35576) | 1 | 1 |
| G: -6323.39516 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.20942 HOMO: -7.05047 LUMO: 1.82044 factor:1 | -1 (0.55144) | 1 | 1 |
| G: -6323.39516 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.86867 HOMO: -6.87632 LUMO: 1.92657 factor:1 | 1 (-0.10781) | 1 | 1 |
| G: -6323.39516 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.75710 HOMO: -6.58788 LUMO: 1.91568 factor:1 | -1 (0.00376) | 1 | -1 |
| G: -6323.39516 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.63536 HOMO: -7.17292 LUMO: 1.90752 factor:1 | -1 (0.12550) | 1 | 1 |
| G: -6323.39516 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.64581 HOMO: -6.93890 LUMO: 1.80684 factor:1 | -1 (0.11505) | 1 | 1 |
| G: -6323.39516 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.80742 HOMO: -7.10761 LUMO: 2.20956 factor:1 | 1 (-0.04656) | 1 | 1 |
| G: -6323.39516 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.69180 HOMO: -6.85727 LUMO: 2.13609 factor:1 | -1 (0.06906) | 1 | -1 |
| G: -6323.39516 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.89811 HOMO: -6.64502 LUMO: 1.38506 factor:1 | 1 (-0.13725) | -1 | -1 |
| G: -6323.39516 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.84276 HOMO: -6.87360 LUMO: 1.15648 factor:1 | 1 (-0.08191) | -1 | -1 |
| G: -6323.39516 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.61158 HOMO: -6.67223 LUMO: 2.07351 factor:1 | -1 (0.14928) | 1 | 1 |
| G: -6323.39516 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.52845 HOMO: -6.29671 LUMO: 2.43270 factor:1 | -1 (0.23241) | -1 | -1 |
| G: -6323.39516 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.53468 HOMO: -6.90897 LUMO: 2.28848 factor:1 | -1 (0.22618) | 1 | 1 |
| G: -6323.39516 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.42469 HOMO: -7.04231 LUMO: 1.70071 factor:1 | -1 (0.33617) | 1 | 1 |
| G: -6323.39516 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.94908 HOMO: -6.69944 LUMO: 1.94834 factor:1 | 1 (-0.18822) | 1 | 1 |
| G: -6323.39516 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.71463 HOMO: -6.56067 LUMO: 2.20956 factor:1 | -1 (0.04623) | -1 | -1 |
| G: -6323.39516 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.59819 HOMO: -6.65046 LUMO: 2.06807 factor:1 | -1 (0.16267) | 1 | -1 |
| G: -6323.39516 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.76663 HOMO: -7.08584 LUMO: 1.98915 factor:1 | 1 (-0.00577) | 1 | 1 |
| G: -6323.39516 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.47653 HOMO: -6.69400 LUMO: 2.09256 factor:1 | -1 (0.28433) | 1 | 1 |
| G: -6323.39516 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.49057 HOMO: -6.62869 LUMO: 2.16331 factor:1 | -1 (0.27029) | 1 | 1 |
| G: -6323.39516 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.34504 HOMO: -6.85183 LUMO: 2.16058 factor:1 | -1 (0.41582) | 1 | 1 |
| G: -6323.39516 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.61500 HOMO: -6.54706 LUMO: 1.92384 factor:1 | -1 (0.14585) | -1 | -1 |
| G: -6323.39516 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.33919 HOMO: -6.84366 LUMO: 2.48984 factor:1 | -1 (0.42167) | 1 | 1 |
| G: -6323.39516 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.33650 HOMO: -6.77291 LUMO: 2.46263 factor:1 | -1 (0.42436) | 1 | 1 |
| G: -6323.39516 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.19353 HOMO: -7.01782 LUMO: 2.31025 factor:1 | -1 (0.56733) | 1 | 1 |
| G: -6323.39516 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.33541 HOMO: -6.94707 LUMO: 2.29664 factor:1 | -1 (0.42545) | 1 | 1 |
| G: -6323.39516 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.20477 HOMO: -6.64230 LUMO: 1.97283 factor:1 | -1 (0.55609) | 1 | 1 |
| G: -6323.39516 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12586.96528 HOMO: -6.47359 LUMO: 2.20412 factor:1 | -1 (0.79558) | -1 | -1 |
| G: -6323.39516 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.44295 HOMO: -6.90625 LUMO: 1.92384 factor:1 | -1 (0.31791) | 1 | 1 |
| G: -6323.39516 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.64031 HOMO: -7.17020 LUMO: 2.06807 factor:1 | -1 (0.12055) | 1 | 1 |
| G: -6323.39516 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.83196 HOMO: -6.65046 LUMO: 2.20956 factor:1 | 1 (-0.07110) | 1 | -1 |
| G: -6323.39516 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.81838 HOMO: -7.07496 LUMO: 1.82861 factor:1 | 1 (-0.05752) | 1 | 1 |
| G: -6323.39516 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.61079 HOMO: -6.83006 LUMO: 2.14970 factor:1 | -1 (0.15007) | 1 | -1 |
| G: -6323.39516 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.80676 HOMO: -6.92802 LUMO: 1.99187 factor:1 | 1 (-0.04591) | 1 | 1 |
| G: -6323.39516 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.81397 HOMO: -6.69672 LUMO: 2.36739 factor:1 | 1 (-0.05312) | 1 | -1 |
| G: -6323.39516 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.91980 HOMO: -7.13755 LUMO: 2.00276 factor:1 | 1 (-0.15894) | 1 | 1 |
| G: -6323.39516 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.69683 HOMO: -6.92530 LUMO: 2.25582 factor:1 | -1 (0.06403) | 1 | 1 |
| G: -6323.39516 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.61838 HOMO: -6.77564 LUMO: 1.97827 factor:1 | -1 (0.14248) | 1 | 1 |
| G: -6323.39516 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.60265 HOMO: -6.87904 LUMO: 1.60003 factor:1 | -1 (0.15821) | 1 | 1 |
| G: -6323.39516 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.46610 HOMO: -6.62869 LUMO: 1.90480 factor:1 | -1 (0.29475) | 1 | 1 |
| G: -6323.39516 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.39862 HOMO: -6.71033 LUMO: 1.54833 factor:1 | -1 (0.36224) | -1 | -1 |
| G: -6323.39516 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.45351 HOMO: -6.74298 LUMO: 1.47486 factor:1 | -1 (0.30735) | -1 | -1 |
| G: -6323.39516 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.47688 HOMO: -6.77019 LUMO: 1.90480 factor:1 | -1 (0.28398) | 1 | 1 |
| G: -6323.39516 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.38599 HOMO: -6.70489 LUMO: 1.99459 factor:1 | -1 (0.37486) | 1 | 1 |
| G: -6323.39516 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.67033 HOMO: -6.73482 LUMO: 2.08711 factor:1 | -1 (0.09053) | 1 | 1 |
| G: -6323.39516 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.66442 HOMO: -6.46543 LUMO: 1.73881 factor:1 | -1 (0.09644) | -1 | -1 |
| G: -6323.39516 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.67767 HOMO: -6.96067 LUMO: 2.26127 factor:1 | -1 (0.08319) | 1 | 1 |
| G: -6323.39516 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.59743 HOMO: -6.67767 LUMO: 2.10616 factor:1 | -1 (0.16343) | 1 | 1 |
| G: -6323.39516 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.35639 HOMO: -6.28855 LUMO: 2.35923 factor:1 | -1 (0.40447) | -1 | -1 |
| G: -6323.39516 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.45541 HOMO: -6.80285 LUMO: 1.62724 factor:1 | -1 (0.30545) | 1 | 1 |
| G: -6323.39516 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.39625 HOMO: -6.85455 LUMO: 2.23133 factor:1 | -1 (0.36461) | 1 | 1 |
| G: -6323.39516 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.25522 HOMO: -6.51713 LUMO: 2.33474 factor:1 | -1 (0.50564) | -1 | -1 |
| G: -6323.39516 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.51952 HOMO: -6.88176 LUMO: 2.15242 factor:1 | -1 (0.24134) | 1 | 1 |
| G: -6323.39516 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.83389 HOMO: -6.54434 LUMO: 2.32113 factor:1 | 1 (-0.07304) | -1 | -1 |
| G: -6323.39516 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.53892 HOMO: -6.62597 LUMO: 2.24222 factor:1 | -1 (0.22194) | 1 | 1 |
| G: -6323.39516 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.59070 HOMO: -6.74570 LUMO: 2.19868 factor:1 | -1 (0.17015) | 1 | 1 |
| G: -6323.39516 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.66608 HOMO: -6.62869 LUMO: 1.98915 factor:1 | -1 (0.09478) | 1 | 1 |
| G: -6323.39516 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.74687 HOMO: -6.64502 LUMO: 2.13881 factor:1 | -1 (0.01399) | 1 | 1 |
| G: -6323.39516 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.70246 HOMO: -6.95795 LUMO: 1.82316 factor:1 | -1 (0.05840) | 1 | 1 |
| G: -6323.39516 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.38719 HOMO: -6.77291 LUMO: 1.36329 factor:1 | -1 (0.37367) | -1 | -1 |
| G: -6323.39516 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.54673 HOMO: -6.45726 LUMO: 1.73064 factor:1 | -1 (0.21413) | -1 | -1 |
| G: -6323.39516 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.38009 HOMO: -6.49264 LUMO: 1.77418 factor:1 | -1 (0.38077) | -1 | -1 |
| G: -6323.39516 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.74995 HOMO: -6.60420 LUMO: 2.20956 factor:1 | -1 (0.01091) | 1 | 1 |
| G: -6323.39516 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.69033 HOMO: -6.56067 LUMO: 2.05718 factor:1 | -1 (0.07053) | -1 | -1 |
| G: -6323.39516 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.63841 HOMO: -6.62597 LUMO: 1.70343 factor:1 | -1 (0.12245) | 1 | 1 |
| G: -6323.39516 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.36512 HOMO: -6.69400 LUMO: 2.16875 factor:1 | -1 (0.39574) | 1 | 1 |
| G: -6323.39516 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.43827 HOMO: -6.63958 LUMO: 2.11977 factor:1 | -1 (0.32259) | 1 | 1 |
| G: -6323.39516 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.30986 HOMO: -6.92802 LUMO: 1.82044 factor:1 | -1 (0.45100) | 1 | -1 |
| G: -6323.39516 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.19628 HOMO: -6.56339 LUMO: 2.30480 factor:1 | -1 (0.56458) | -1 | -1 |
| G: -6323.39516 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12586.98457 HOMO: -6.63958 LUMO: 1.91024 factor:1 | -1 (0.77629) | 1 | -1 |
| G: -6323.39516 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.52787 HOMO: -6.93074 LUMO: 2.05446 factor:1 | -1 (0.23298) | 1 | 1 |
| G: -6323.39516 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12587.40319 HOMO: -6.61509 LUMO: 2.03813 factor:1 | -1 (0.35767) | 1 | 1 |
| G: -7301.27697 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -13565.47989 HOMO: -6.61237 LUMO: 1.91296 factor:1 | -1 (0.16278) | 1 | -1 |
| G: -7301.27697 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -13565.48261 HOMO: -6.86815 LUMO: 1.95378 factor:1 | -1 (0.16006) | 1 | 1 |
| G: -7301.27697 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -13565.49227 HOMO: -6.63686 LUMO: 1.70888 factor:1 | -1 (0.15040) | 1 | 1 |
| G: -7301.27697 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -13565.10429 HOMO: -6.57971 LUMO: 2.20140 factor:1 | -1 (0.53838) | 1 | -1 |
| G: -7301.27697 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -13565.13213 HOMO: -6.41100 LUMO: 1.96738 factor:1 | -1 (0.51054) | -1 | -1 |
| G: -7301.27697 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -13565.50082 HOMO: -6.90081 LUMO: 1.65989 factor:1 | -1 (0.14185) | 1 | 1 |
| G: -7301.27697 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -13564.95838 HOMO: -6.68312 LUMO: 1.97827 factor:1 | -1 (0.68428) | 1 | -1 |
| G: -7301.27697 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -13565.00434 HOMO: -6.65318 LUMO: 2.10888 factor:1 | -1 (0.63832) | 1 | -1 |
| G: -7301.27697 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -13565.22884 HOMO: -6.62053 LUMO: 2.28848 factor:1 | -1 (0.41383) | 1 | -1 |
| G: -7301.27697 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -13565.28960 HOMO: -6.65863 LUMO: 2.29664 factor:1 | -1 (0.35307) | 1 | -1 |
| G: -7301.27697 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -13565.19537 HOMO: -6.63958 LUMO: 2.07623 factor:1 | -1 (0.44730) | 1 | -1 |
| G: -7301.27697 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -13565.32010 HOMO: -6.58243 LUMO: 2.20684 factor:1 | -1 (0.32256) | 1 | 1 |
| G: -7301.27697 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -13565.14922 HOMO: -6.59332 LUMO: 2.05174 factor:1 | -1 (0.49345) | 1 | -1 |
| G: -7301.27697 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -13565.21891 HOMO: -6.95251 LUMO: 2.20140 factor:1 | -1 (0.42376) | 1 | 1 |
| G: -7301.66678 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -13565.47989 HOMO: -6.84638 LUMO: 2.39732 factor:1 | -1 (0.55258) | 1 | 1 |
| G: -7301.66678 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -13565.48261 HOMO: -6.86815 LUMO: 2.47896 factor:1 | -1 (0.54986) | 1 | 1 |
| G: -7301.66678 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -13565.49227 HOMO: -7.00693 LUMO: 2.43270 factor:1 | -1 (0.54020) | 1 | 1 |
| G: -7301.66678 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -13565.10429 HOMO: -6.58788 LUMO: 2.30208 factor:1 | -1 (0.92818) | 1 | 1 |
| G: -7301.66678 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -13565.13213 HOMO: -6.63958 LUMO: 2.28031 factor:1 | -1 (0.90034) | 1 | 1 |
| G: -7301.66678 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -13565.50082 HOMO: -6.74570 LUMO: 2.28304 factor:1 | -1 (0.53166) | 1 | 1 |
| G: -7301.66678 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -13564.95838 HOMO: -6.78380 LUMO: 2.16331 factor:1 | -1 (1.07409) | 1 | 1 |
| G: -7301.66678 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -13565.00434 HOMO: -6.52529 LUMO: 2.05718 factor:1 | -1 (1.02813) | -1 | -1 |
| G: -7301.66678 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -13565.22884 HOMO: -6.41644 LUMO: 1.65445 factor:1 | -1 (0.80363) | -1 | -1 |
| G: -7301.66678 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -13565.28960 HOMO: -6.34570 LUMO: 1.22451 factor:1 | -1 (0.74287) | -1 | -1 |
| G: -7301.66678 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -13565.19537 HOMO: -6.14433 LUMO: 1.85582 factor:1 | -1 (0.83710) | -1 | -1 |
| G: -7301.66678 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -13565.32010 HOMO: -6.62053 LUMO: 1.92112 factor:1 | -1 (0.71237) | 1 | -1 |
| G: -7301.66678 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -13565.14922 HOMO: -6.63414 LUMO: 1.61908 factor:1 | -1 (0.88325) | 1 | 1 |
| G: -7301.66678 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -13565.21891 HOMO: -6.75931 LUMO: 1.87214 factor:1 | -1 (0.81357) | 1 | 1 |
| G: -7302.20847 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -13565.47989 HOMO: -6.55794 LUMO: 1.77418 factor:1 | -1 (1.09428) | -1 | -1 |
| G: -7302.20847 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -13565.48261 HOMO: -6.52801 LUMO: 1.82044 factor:1 | -1 (1.09156) | -1 | -1 |
| G: -7302.20847 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -13565.49227 HOMO: -6.77564 LUMO: 1.97827 factor:1 | -1 (1.08190) | 1 | 1 |
| G: -7302.20847 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -13565.10429 HOMO: -6.93890 LUMO: 1.81228 factor:1 | -1 (1.46988) | 1 | 1 |
| G: -7302.20847 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -13565.13213 HOMO: -6.85455 LUMO: 1.75513 factor:1 | -1 (1.44204) | 1 | 1 |
| G: -7302.20847 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -13565.50082 HOMO: -6.86815 LUMO: 1.64629 factor:1 | -1 (1.07335) | 1 | 1 |
| G: -7302.20847 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -13564.95838 HOMO: -6.98516 LUMO: 1.84765 factor:1 | -1 (1.61578) | 1 | 1 |
| G: -7302.20847 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -13565.00434 HOMO: -6.04637 LUMO: 1.94017 factor:1 | -1 (1.56982) | -1 | -1 |
| G: -7302.20847 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -13565.22884 HOMO: -6.86271 LUMO: 2.11977 factor:1 | -1 (1.34533) | 1 | -1 |
| G: -7302.20847 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -13565.28960 HOMO: -6.72938 LUMO: 2.11160 factor:1 | -1 (1.28457) | 1 | -1 |
| G: -7302.20847 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -13565.19537 HOMO: -7.01782 LUMO: 2.13609 factor:1 | -1 (1.37880) | 1 | 1 |
| G: -7302.20847 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -13565.32010 HOMO: -6.18515 LUMO: 2.04630 factor:1 | -1 (1.25406) | -1 | -1 |
| G: -7302.20847 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -13565.14922 HOMO: -6.60965 LUMO: 2.17147 factor:1 | -1 (1.42495) | 1 | -1 |
| G: -7302.20847 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -13565.21891 HOMO: -6.87360 LUMO: 2.35378 factor:1 | -1 (1.35526) | 1 | 1 |
| G: -7300.17736 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -13565.47989 HOMO: -6.72938 LUMO: 2.20140 factor:1 | 1 (-0.93683) | 1 | -1 |
| G: -7300.17736 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -13565.48261 HOMO: -6.88448 LUMO: 2.54154 factor:1 | 1 (-0.93955) | 1 | -1 |
| G: -7300.17736 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -13565.49227 HOMO: -6.87087 LUMO: 2.16058 factor:1 | 1 (-0.94921) | 1 | 1 |
| G: -7300.17736 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -13565.10429 HOMO: -7.11306 LUMO: 2.04085 factor:1 | 1 (-0.56123) | 1 | 1 |
| G: -7300.17736 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -13565.13213 HOMO: -6.66951 LUMO: 1.68438 factor:1 | 1 (-0.58907) | 1 | 1 |
| G: -7300.17736 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -13565.50082 HOMO: -7.08312 LUMO: 2.19324 factor:1 | 1 (-0.95776) | 1 | 1 |
| G: -7300.17736 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -13564.95838 HOMO: -6.69128 LUMO: 2.13881 factor:1 | 1 (-0.41533) | 1 | -1 |
| G: -7300.17736 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -13565.00434 HOMO: -6.80285 LUMO: 2.16603 factor:1 | 1 (-0.46129) | 1 | 1 |
| G: -7300.17736 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -13565.22884 HOMO: -6.82189 LUMO: 2.46807 factor:1 | 1 (-0.68578) | 1 | 1 |
| G: -7300.17736 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -13565.28960 HOMO: -6.78652 LUMO: 2.12521 factor:1 | 1 (-0.74654) | 1 | 1 |
| G: -7300.17736 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -13565.19537 HOMO: -6.47903 LUMO: 1.70071 factor:1 | 1 (-0.65231) | -1 | -1 |
| G: -7300.17736 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -13565.32010 HOMO: -6.37019 LUMO: 1.24356 factor:1 | 1 (-0.77705) | -1 | -1 |
| G: -7300.17736 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -13565.14922 HOMO: -6.69400 LUMO: 1.67350 factor:1 | 1 (-0.60616) | 1 | 1 |
| G: -7300.17736 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -13565.21891 HOMO: -7.51851 LUMO: 0.27756 factor:1 | 1 (-0.67585) | -1 | -1 |
| G: -7300.24164 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -13565.47989 HOMO: -6.95795 LUMO: -0.72110 factor:1 | 1 (-0.87256) | -1 | -1 |
| G: -7300.24164 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -13565.48261 HOMO: -6.88720 LUMO: -0.67484 factor:1 | 1 (-0.87528) | -1 | -1 |
| G: -7300.24164 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -13565.49227 HOMO: -6.83550 LUMO: -0.57144 factor:1 | 1 (-0.88494) | -1 | -1 |
| G: -7300.24164 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -13565.10429 HOMO: -6.80285 LUMO: -0.57144 factor:1 | 1 (-0.49696) | -1 | -1 |
| G: -7300.24164 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -13565.13213 HOMO: -6.76475 LUMO: -0.53062 factor:1 | 1 (-0.52480) | -1 | -1 |
| G: -7300.24164 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -13565.50082 HOMO: -6.66951 LUMO: 1.74969 factor:1 | 1 (-0.89349) | 1 | 1 |
| G: -7300.24164 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -13564.95838 HOMO: -6.53345 LUMO: 1.89935 factor:1 | 1 (-0.35105) | -1 | -1 |
| G: -7300.24164 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -13565.00434 HOMO: -6.65046 LUMO: 2.01364 factor:1 | 1 (-0.39701) | 1 | -1 |
| G: -7300.24164 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -13565.22884 HOMO: -6.64230 LUMO: 2.11977 factor:1 | 1 (-0.62151) | 1 | -1 |
| G: -7300.24164 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -13565.28960 HOMO: -6.44910 LUMO: 2.13337 factor:1 | 1 (-0.68227) | -1 | -1 |
| G: -7300.24164 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -13565.19537 HOMO: -7.05591 LUMO: 1.98915 factor:1 | 1 (-0.58804) | 1 | -1 |
| G: -7300.24164 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -13565.32010 HOMO: -7.02326 LUMO: 2.49256 factor:1 | 1 (-0.71278) | 1 | 1 |
| G: -7300.24164 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -13565.14922 HOMO: -6.32937 LUMO: 2.51161 factor:1 | 1 (-0.54189) | -1 | -1 |
| G: -7300.24164 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -13565.21891 HOMO: -6.96067 LUMO: 2.20140 factor:1 | 1 (-0.61158) | 1 | 1 |
| G: -7301.83364 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -13565.47989 HOMO: -6.97972 LUMO: 2.55243 factor:1 | -1 (0.71944) | 1 | 1 |
| G: -7301.83364 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -13565.48261 HOMO: -6.72665 LUMO: 2.46535 factor:1 | -1 (0.71672) | 1 | 1 |
| G: -7301.83364 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -13565.49227 HOMO: -6.41917 LUMO: 2.35106 factor:1 | -1 (0.70706) | -1 | -1 |
| G: -7301.83364 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -13565.10429 HOMO: -6.75114 LUMO: 2.32929 factor:1 | -1 (1.09504) | 1 | 1 |
| G: -7301.83364 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -13565.13213 HOMO: -6.91713 LUMO: 2.27215 factor:1 | -1 (1.06720) | 1 | 1 |
| G: -7301.83364 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -13565.50082 HOMO: -6.54978 LUMO: 2.00276 factor:1 | -1 (0.69852) | -1 | -1 |
| G: -7301.83364 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -13564.95838 HOMO: -6.62325 LUMO: 2.05990 factor:1 | -1 (1.24095) | 1 | 1 |
| G: -7301.83364 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -13565.00434 HOMO: -6.86271 LUMO: 2.14970 factor:1 | -1 (1.19499) | 1 | 1 |
| G: -7301.83364 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -13565.22884 HOMO: -6.77564 LUMO: 2.25855 factor:1 | -1 (0.97049) | 1 | -1 |
| G: -7301.83364 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -13565.28960 HOMO: -6.71305 LUMO: 1.94561 factor:1 | -1 (0.90973) | 1 | -1 |
| G: -7301.83364 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -13565.19537 HOMO: -6.75659 LUMO: 1.94561 factor:1 | -1 (1.00396) | 1 | -1 |
| G: -7301.83364 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -13565.32010 HOMO: -6.94979 LUMO: 2.33474 factor:1 | -1 (0.87923) | 1 | -1 |
| G: -7301.83364 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -13565.14922 HOMO: -6.85727 LUMO: 2.50345 factor:1 | -1 (1.05011) | 1 | -1 |
| G: -7301.83364 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -13565.21891 HOMO: -6.87360 LUMO: 2.43270 factor:1 | -1 (0.98043) | 1 | -1 |
| G: -7300.89977 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -13565.47989 HOMO: -6.57427 LUMO: 2.46807 factor:1 | 1 (-0.21443) | 1 | -1 |
| G: -7300.89977 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -13565.48261 HOMO: -7.16204 LUMO: 2.15242 factor:1 | 1 (-0.21715) | 1 | 1 |
| G: -7300.89977 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -13565.49227 HOMO: -6.62869 LUMO: 2.11432 factor:1 | 1 (-0.22681) | 1 | -1 |
| G: -7300.89977 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -13565.10429 HOMO: -7.05591 LUMO: 2.26671 factor:1 | -1 (0.16117) | 1 | -1 |
| G: -7300.89977 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -13565.13213 HOMO: -7.13483 LUMO: 1.47758 factor:1 | -1 (0.13334) | -1 | -1 |
| G: -7300.89977 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -13565.50082 HOMO: -6.72938 LUMO: 1.57282 factor:1 | 1 (-0.23535) | -1 | -1 |
| G: -7300.89977 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -13564.95838 HOMO: -6.17426 LUMO: 1.81228 factor:1 | -1 (0.30708) | -1 | -1 |
| G: -7300.89977 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -13565.00434 HOMO: -6.65318 LUMO: 1.93473 factor:1 | -1 (0.26112) | 1 | -1 |
| G: -7300.89977 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -13565.22884 HOMO: -6.18515 LUMO: 2.01364 factor:1 | -1 (0.03663) | -1 | -1 |
| G: -7300.89977 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -13565.28960 HOMO: -7.05591 LUMO: 2.13337 factor:1 | 1 (-0.02414) | 1 | 1 |
| G: -7300.89977 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -13565.19537 HOMO: -6.90897 LUMO: 2.29664 factor:1 | -1 (0.07010) | 1 | -1 |
| G: -7300.89977 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -13565.32010 HOMO: -7.11034 LUMO: 2.17147 factor:1 | 1 (-0.05464) | 1 | 1 |
| G: -7300.89977 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -13565.14922 HOMO: -6.82734 LUMO: 2.26671 factor:1 | -1 (0.11625) | 1 | 1 |
| G: -7300.89977 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -13565.21891 HOMO: -6.34842 LUMO: 2.34562 factor:1 | -1 (0.04656) | -1 | -1 |
| G: -7301.15060 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -13565.47989 HOMO: -6.62053 LUMO: 2.22861 factor:1 | -1 (0.03641) | 1 | -1 |
| G: -7301.15060 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -13565.48261 HOMO: -6.80557 LUMO: 2.07079 factor:1 | -1 (0.03369) | 1 | -1 |
| G: -7301.15060 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -13565.49227 HOMO: -6.60692 LUMO: 2.46263 factor:1 | -1 (0.02403) | 1 | -1 |
| G: -7301.15060 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -13565.10429 HOMO: -7.02054 LUMO: 2.08711 factor:1 | -1 (0.41201) | 1 | -1 |
| G: -7301.15060 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -13565.13213 HOMO: -6.78652 LUMO: 2.02453 factor:1 | -1 (0.38417) | 1 | 1 |
| G: -7301.15060 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -13565.50082 HOMO: -6.51168 LUMO: 2.06534 factor:1 | -1 (0.01548) | -1 | -1 |
| G: -7301.15060 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -13564.95838 HOMO: -6.50080 LUMO: 2.01636 factor:1 | -1 (0.55792) | -1 | -1 |
| G: -7301.15060 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -13565.00434 HOMO: -6.54434 LUMO: 1.84493 factor:1 | -1 (0.51196) | -1 | -1 |
| G: -7301.15060 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -13565.22884 HOMO: -6.47087 LUMO: 1.76330 factor:1 | -1 (0.28746) | -1 | -1 |
| G: -7301.15060 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -13565.28960 HOMO: -6.78924 LUMO: 2.39460 factor:1 | -1 (0.22670) | 1 | 1 |
| G: -7301.15060 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -13565.19537 HOMO: -6.59876 LUMO: 1.84493 factor:1 | -1 (0.32093) | 1 | 1 |
| G: -7301.15060 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -13565.32010 HOMO: -6.41644 LUMO: 2.05174 factor:1 | -1 (0.19619) | -1 | -1 |
| G: -7301.15060 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -13565.14922 HOMO: -6.52257 LUMO: 2.11160 factor:1 | -1 (0.36708) | -1 | -1 |
| G: -7301.15060 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -13565.21891 HOMO: -6.90897 LUMO: 2.34018 factor:1 | -1 (0.29739) | 1 | 1 |
| G: -7300.19521 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -13565.47989 HOMO: -6.97428 LUMO: 1.86126 factor:1 | 1 (-0.91898) | 1 | 1 |
| G: -7300.19521 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -13565.48261 HOMO: -7.13483 LUMO: 2.14698 factor:1 | 1 (-0.92170) | 1 | -1 |
| G: -7300.19521 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -13565.49227 HOMO: -7.16748 LUMO: 2.31841 factor:1 | 1 (-0.93136) | 1 | 1 |
| G: -7300.19521 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -13565.10429 HOMO: -6.87087 LUMO: 2.38916 factor:1 | 1 (-0.54338) | 1 | -1 |
| G: -7300.19521 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -13565.13213 HOMO: -6.93074 LUMO: 2.42181 factor:1 | 1 (-0.57122) | 1 | -1 |
| G: -7300.19521 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -13565.50082 HOMO: -6.90081 LUMO: 2.00276 factor:1 | 1 (-0.93991) | 1 | -1 |
| G: -7300.19521 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -13564.95838 HOMO: -6.99333 LUMO: 2.03541 factor:1 | 1 (-0.39748) | 1 | 1 |
| G: -7300.19521 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -13565.00434 HOMO: -6.89264 LUMO: 1.57554 factor:1 | 1 (-0.44344) | -1 | -1 |
| G: -7300.19521 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -13565.22884 HOMO: -6.48175 LUMO: 1.85854 factor:1 | 1 (-0.66793) | -1 | -1 |
| G: -7300.19521 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -13565.28960 HOMO: -6.69400 LUMO: 1.62452 factor:1 | 1 (-0.72869) | 1 | 1 |
| G: -7300.19521 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -13565.19537 HOMO: -6.50896 LUMO: 1.88303 factor:1 | 1 (-0.63446) | -1 | -1 |
| G: -7300.19521 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -13565.32010 HOMO: -6.60420 LUMO: 2.05990 factor:1 | 1 (-0.75920) | 1 | 1 |
| G: -7300.19521 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -13565.14922 HOMO: -7.14299 LUMO: 2.07351 factor:1 | 1 (-0.58831) | 1 | 1 |
| G: -7300.19521 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -13565.21891 HOMO: -7.06408 LUMO: 1.81228 factor:1 | 1 (-0.65800) | 1 | 1 |
| G: -7300.87727 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -13565.47989 HOMO: -6.67495 LUMO: 1.79595 factor:1 | 1 (-0.23693) | 1 | 1 |
| G: -7300.87727 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -13565.48261 HOMO: -6.45182 LUMO: 2.15786 factor:1 | 1 (-0.23965) | -1 | -1 |
| G: -7300.87727 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -13565.49227 HOMO: -6.93346 LUMO: 2.45719 factor:1 | 1 (-0.24931) | 1 | 1 |
| G: -7300.87727 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -13565.10429 HOMO: -6.50080 LUMO: 2.08167 factor:1 | -1 (0.13867) | -1 | -1 |
| G: -7300.87727 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -13565.13213 HOMO: -6.83550 LUMO: -0.67484 factor:1 | -1 (0.11083) | -1 | -1 |
| G: -7300.87727 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -13565.50082 HOMO: -7.04231 LUMO: 0.54151 factor:1 | 1 (-0.25786) | -1 | -1 |
| G: -7300.87727 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -13564.95838 HOMO: -6.79740 LUMO: 1.91296 factor:1 | -1 (0.28458) | -1 | -1 |
| G: -7300.87727 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -13565.00434 HOMO: -7.35796 LUMO: -1.04220 factor:1 | -1 (0.23862) | -1 | -1 |
| G: -7300.87727 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -13565.22884 HOMO: -6.62597 LUMO: -0.44082 factor:1 | -1 (0.01412) | -1 | -1 |
| G: -7300.87727 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -13565.28960 HOMO: -6.45182 LUMO: -0.20409 factor:1 | 1 (-0.04664) | -1 | -1 |
| G: -7300.87727 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -13565.19537 HOMO: -6.51168 LUMO: -0.23130 factor:1 | -1 (0.04759) | -1 | -1 |
| G: -7300.87727 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -13565.32010 HOMO: -7.14027 LUMO: 0.49797 factor:1 | 1 (-0.07714) | -1 | -1 |
| G: -7300.87727 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -13565.14922 HOMO: -7.55660 LUMO: 0.24762 factor:1 | -1 (0.09374) | -1 | -1 |
| G: -7300.87727 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -13565.21891 HOMO: -6.88992 LUMO: -0.64763 factor:1 | -1 (0.02405) | -1 | -1 |
| G: -5345.34143 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11610.46015 HOMO: -6.72665 LUMO: -0.45987 factor:1 | 1 (-0.75302) | -1 | -1 |
| G: -5345.34143 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11610.39288 HOMO: -6.72121 LUMO: -0.58232 factor:1 | 1 (-0.68575) | -1 | -1 |
| G: -5345.34143 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11610.19614 HOMO: -7.26816 LUMO: 0.32926 factor:1 | 1 (-0.48902) | -1 | -1 |
| G: -5345.34143 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11610.32518 HOMO: -6.57155 LUMO: -0.53606 factor:1 | 1 (-0.61805) | -1 | -1 |
| G: -5345.34143 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11610.40232 HOMO: -6.50896 LUMO: -0.43810 factor:1 | 1 (-0.69520) | -1 | -1 |
| G: -5345.34143 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11610.22809 HOMO: -6.73210 LUMO: -0.51430 factor:1 | 1 (-0.52096) | -1 | -1 |
| G: -5345.34143 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11610.44472 HOMO: -6.77019 LUMO: -0.62858 factor:1 | 1 (-0.73759) | -1 | -1 |
| G: -5345.34143 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11610.33541 HOMO: -6.82462 LUMO: -0.67484 factor:1 | 1 (-0.62828) | -1 | -1 |
| G: -5345.34143 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11610.33829 HOMO: -6.79740 LUMO: -0.55511 factor:1 | 1 (-0.63117) | -1 | -1 |
| G: -5345.34143 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11610.46793 HOMO: -6.79740 LUMO: -0.67756 factor:1 | 1 (-0.76080) | -1 | -1 |
| G: -5345.34143 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11610.37819 HOMO: -6.75114 LUMO: -0.55239 factor:1 | 1 (-0.67106) | -1 | -1 |
| G: -5345.34143 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11610.48050 HOMO: -6.49536 LUMO: -0.25307 factor:1 | 1 (-0.77337) | -1 | -1 |
| G: -5345.34143 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11610.27761 HOMO: -6.48992 LUMO: -0.25034 factor:1 | 1 (-0.57049) | -1 | -1 |
| G: -5345.34143 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11610.20224 HOMO: -6.52801 LUMO: -0.28028 factor:1 | 1 (-0.49511) | -1 | -1 |
| G: -5345.34143 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11610.41351 HOMO: -7.22462 LUMO: 0.52518 factor:1 | 1 (-0.70638) | -1 | -1 |
| G: -5345.34143 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11610.28352 HOMO: -6.59332 LUMO: -0.27211 factor:1 | 1 (-0.57639) | -1 | -1 |
| G: -5345.34143 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11610.03230 HOMO: -6.57427 LUMO: -0.16871 factor:1 | 1 (-0.32518) | -1 | -1 |
| G: -5345.34143 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11610.15867 HOMO: -6.71033 LUMO: 1.59187 factor:1 | 1 (-0.45155) | -1 | -1 |
| G: -5345.34143 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11610.03559 HOMO: -6.72121 LUMO: 2.00004 factor:1 | 1 (-0.32847) | -1 | -1 |
| G: -5345.34143 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11610.19018 HOMO: -6.61509 LUMO: 1.55921 factor:1 | 1 (-0.48306) | -1 | -1 |
| G: -5345.34143 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11610.08047 HOMO: -6.55250 LUMO: 1.73064 factor:1 | 1 (-0.37334) | -1 | -1 |
| G: -5345.34143 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11610.34978 HOMO: -6.66135 LUMO: 2.02181 factor:1 | 1 (-0.64265) | -1 | -1 |
| G: -5345.34143 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11610.16871 HOMO: -6.84911 LUMO: 1.98099 factor:1 | 1 (-0.46159) | -1 | -1 |
| G: -5345.34143 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11610.32183 HOMO: -6.66679 LUMO: 1.98371 factor:1 | 1 (-0.61471) | -1 | -1 |
| G: -5345.34143 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11610.19024 HOMO: -6.67495 LUMO: 2.04085 factor:1 | 1 (-0.48311) | -1 | -1 |
| G: -5345.34143 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11610.14953 HOMO: -6.89809 LUMO: 1.95106 factor:1 | 1 (-0.44240) | -1 | -1 |
| G: -5345.34143 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11610.49574 HOMO: -6.50352 LUMO: 1.88847 factor:1 | 1 (-0.78861) | -1 | -1 |
| G: -5345.34143 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11610.19609 HOMO: -6.93618 LUMO: 2.00004 factor:1 | 1 (-0.48896) | -1 | -1 |
| G: -5345.34143 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11609.86596 HOMO: -6.50896 LUMO: 1.73609 factor:1 | 1 (-0.15883) | -1 | -1 |
| G: -5345.34143 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11610.05053 HOMO: -6.69672 LUMO: 2.37283 factor:1 | 1 (-0.34341) | -1 | -1 |
| G: -5345.34143 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11610.08131 HOMO: -6.65591 LUMO: 2.20684 factor:1 | 1 (-0.37418) | -1 | -1 |
| G: -5345.34143 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11610.29005 HOMO: -6.23957 LUMO: 1.78507 factor:1 | 1 (-0.58292) | -1 | -1 |
| G: -5345.34143 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11610.14599 HOMO: -6.35114 LUMO: 1.92112 factor:1 | 1 (-0.43887) | -1 | -1 |
| G: -5345.34143 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11609.92182 HOMO: -6.53617 LUMO: 1.75241 factor:1 | 1 (-0.21470) | -1 | -1 |
| G: -5345.34143 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11609.89121 HOMO: -6.60420 LUMO: 1.78779 factor:1 | 1 (-0.18409) | -1 | -1 |
| G: -5345.34143 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11610.11658 HOMO: -7.40422 LUMO: -0.97145 factor:1 | 1 (-0.40945) | -1 | -1 |
| G: -5345.34143 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11610.17854 HOMO: -6.80013 LUMO: -0.69117 factor:1 | 1 (-0.47141) | -1 | -1 |
| G: -5345.34143 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11610.09864 HOMO: -6.68040 LUMO: -0.47076 factor:1 | 1 (-0.39152) | -1 | -1 |
| G: -5345.34143 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11610.25282 HOMO: -7.20285 LUMO: -0.66124 factor:1 | 1 (-0.54570) | -1 | -1 |
| G: -5345.34143 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11610.17445 HOMO: -6.82734 LUMO: -0.60137 factor:1 | 1 (-0.46733) | -1 | -1 |
| G: -5345.34143 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11610.06705 HOMO: -7.18653 LUMO: 0.59321 factor:1 | 1 (-0.35993) | -1 | -1 |
| G: -5345.34143 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11610.38050 HOMO: -7.29265 LUMO: 0.48164 factor:1 | 1 (-0.67337) | -1 | -1 |
| G: -5345.34143 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11609.81532 HOMO: -6.63414 LUMO: -0.25034 factor:1 | 1 (-0.10819) | -1 | -1 |
| G: -5345.34143 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11609.86971 HOMO: -7.20285 LUMO: 0.53879 factor:1 | 1 (-0.16259) | -1 | -1 |
| G: -5345.34143 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11609.82174 HOMO: -6.46815 LUMO: -0.21769 factor:1 | 1 (-0.11461) | -1 | -1 |
| G: -5345.34143 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11610.17728 HOMO: -6.57971 LUMO: -0.18776 factor:1 | 1 (-0.47016) | -1 | -1 |
| G: -5345.34143 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11610.16615 HOMO: -6.90897 LUMO: 1.91296 factor:1 | 1 (-0.45903) | -1 | -1 |
| G: -5345.34143 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11610.11524 HOMO: -6.67495 LUMO: 2.04358 factor:1 | 1 (-0.40812) | -1 | -1 |
| G: -5345.34143 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11610.37451 HOMO: -6.94162 LUMO: 1.73881 factor:1 | 1 (-0.66739) | -1 | -1 |
| G: -5345.34143 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11610.28776 HOMO: -6.73482 LUMO: 1.95922 factor:1 | 1 (-0.58064) | -1 | -1 |
| G: -5345.34143 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11610.34627 HOMO: -6.70489 LUMO: 2.04358 factor:1 | 1 (-0.63914) | -1 | -1 |
| G: -5345.34143 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11610.01929 HOMO: -7.04231 LUMO: 1.79323 factor:1 | 1 (-0.31217) | -1 | -1 |
| G: -5345.34143 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11610.14224 HOMO: -6.68584 LUMO: 1.60275 factor:1 | 1 (-0.43511) | -1 | -1 |
| G: -5345.34143 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11610.01021 HOMO: -6.40556 LUMO: 1.45581 factor:1 | 1 (-0.30308) | -1 | -1 |
| G: -5345.34143 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11609.87540 HOMO: -6.94979 LUMO: 2.16603 factor:1 | 1 (-0.16828) | -1 | -1 |
| G: -5345.34143 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11610.16009 HOMO: -6.84911 LUMO: 1.89935 factor:1 | 1 (-0.45296) | -1 | -1 |
| G: -5345.34143 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11609.95641 HOMO: -6.22052 LUMO: 1.57282 factor:1 | 1 (-0.24928) | -1 | -1 |
| G: -5345.34143 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11609.97616 HOMO: -6.51168 LUMO: 2.10072 factor:1 | 1 (-0.26904) | -1 | -1 |
| G: -5345.34143 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11610.11252 HOMO: -7.03686 LUMO: 2.12249 factor:1 | 1 (-0.40540) | -1 | -1 |
| G: -5345.34143 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11610.11723 HOMO: -6.84094 LUMO: 1.63268 factor:1 | 1 (-0.41010) | -1 | -1 |
| G: -5345.34143 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11609.87488 HOMO: -6.75387 LUMO: 1.72248 factor:1 | 1 (-0.16776) | -1 | -1 |
| G: -5345.34143 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11609.71496 HOMO: -6.86271 LUMO: 1.68711 factor:1 | 1 (-0.00784) | -1 | -1 |
| G: -5345.34143 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11610.25609 HOMO: -6.84094 LUMO: 2.02997 factor:1 | 1 (-0.54896) | -1 | -1 |
| G: -5345.34143 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11610.26847 HOMO: -6.80557 LUMO: 2.02725 factor:1 | 1 (-0.56134) | -1 | -1 |
| G: -5345.34143 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11610.25726 HOMO: -6.38651 LUMO: 1.53472 factor:1 | 1 (-0.55013) | -1 | -1 |
| G: -5345.34143 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11610.55950 HOMO: -7.51306 LUMO: 0.28572 factor:1 | 1 (-0.85237) | -1 | -1 |
| G: -5345.34143 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11610.27750 HOMO: -6.97972 LUMO: -0.74287 factor:1 | 1 (-0.57038) | -1 | -1 |
| G: -5345.34143 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11610.05668 HOMO: -6.83822 LUMO: -0.65852 factor:1 | 1 (-0.34956) | -1 | -1 |
| G: -5345.34143 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11610.28020 HOMO: -6.71305 LUMO: -0.49525 factor:1 | 1 (-0.57307) | -1 | -1 |
| G: -5345.34143 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11610.25345 HOMO: -6.60692 LUMO: -0.22313 factor:1 | 1 (-0.54632) | -1 | -1 |
| G: -5345.34143 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11610.24047 HOMO: -7.20013 LUMO: 0.55239 factor:1 | 1 (-0.53334) | -1 | -1 |
| G: -5345.34143 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11610.15372 HOMO: -6.60420 LUMO: -0.28028 factor:1 | 1 (-0.44659) | -1 | -1 |
| G: -5345.34143 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11610.50673 HOMO: -6.69128 LUMO: -0.30477 factor:1 | 1 (-0.79961) | -1 | -1 |
| G: -5345.34143 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11609.96751 HOMO: -6.65591 LUMO: -0.25579 factor:1 | 1 (-0.26039) | -1 | -1 |
| G: -5345.34143 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11609.84860 HOMO: -6.69128 LUMO: 1.70888 factor:1 | 1 (-0.14147) | -1 | -1 |
| G: -5345.34143 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11610.30618 HOMO: -6.50080 LUMO: 1.87759 factor:1 | 1 (-0.59906) | -1 | -1 |
| G: -5345.34143 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11610.20618 HOMO: -6.85727 LUMO: 1.99187 factor:1 | 1 (-0.49906) | -1 | -1 |
| G: -5345.34143 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11610.13051 HOMO: -6.58788 LUMO: 1.79051 factor:1 | 1 (-0.42338) | -1 | -1 |
| G: -5345.34143 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11610.23707 HOMO: -6.64230 LUMO: 2.16058 factor:1 | 1 (-0.52994) | -1 | -1 |
| G: -5345.34143 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11610.26311 HOMO: -6.58788 LUMO: 2.10616 factor:1 | 1 (-0.55598) | -1 | -1 |
| G: -5345.34143 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11610.41620 HOMO: -7.01782 LUMO: 2.13609 factor:1 | 1 (-0.70907) | -1 | -1 |
| G: -5345.34143 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11610.26063 HOMO: -6.31304 LUMO: 2.31841 factor:1 | 1 (-0.55351) | -1 | -1 |
| G: -5345.34143 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11610.15424 HOMO: -6.94979 LUMO: 2.07895 factor:1 | 1 (-0.44711) | -1 | -1 |
| G: -5345.34143 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11609.99440 HOMO: -6.88992 LUMO: 2.28031 factor:1 | 1 (-0.28727) | -1 | -1 |
| G: -5345.34143 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11609.92346 HOMO: -6.66407 LUMO: 2.07623 factor:1 | 1 (-0.21633) | -1 | -1 |
| G: -5345.34143 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11609.88335 HOMO: -6.52529 LUMO: 1.70071 factor:1 | 1 (-0.17622) | -1 | -1 |
| G: -5345.34143 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11609.78201 HOMO: -6.58788 LUMO: 1.57282 factor:1 | 1 (-0.07489) | -1 | -1 |
| G: -5345.34143 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11610.15486 HOMO: -6.55250 LUMO: 1.95378 factor:1 | 1 (-0.44774) | -1 | -1 |
| G: -5345.34143 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11610.10692 HOMO: -6.24773 LUMO: 1.77962 factor:1 | 1 (-0.39979) | -1 | -1 |
| G: -5345.34143 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11609.92781 HOMO: -6.31304 LUMO: 2.18507 factor:1 | 1 (-0.22068) | -1 | -1 |
| G: -5345.34143 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11610.13135 HOMO: -6.18243 LUMO: 2.01636 factor:1 | 1 (-0.42423) | -1 | -1 |
| G: -5345.34143 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11610.09598 HOMO: -6.99877 LUMO: 2.14970 factor:1 | 1 (-0.38885) | -1 | -1 |
| G: -5345.34143 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11610.12313 HOMO: -6.72665 LUMO: 2.07079 factor:1 | 1 (-0.41601) | -1 | -1 |
| G: -5345.34143 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11610.25592 HOMO: -6.36202 LUMO: 2.17419 factor:1 | 1 (-0.54880) | -1 | -1 |
| G: -5345.34143 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11610.02115 HOMO: -6.78652 LUMO: 2.05718 factor:1 | 1 (-0.31402) | -1 | -1 |
| G: -5345.34143 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11610.14732 HOMO: -6.87360 LUMO: 2.34290 factor:1 | 1 (-0.44020) | -1 | -1 |
| G: -5345.34143 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11610.03222 HOMO: -6.62053 LUMO: 1.89391 factor:1 | 1 (-0.32509) | -1 | -1 |
| G: -5345.34143 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11610.46102 HOMO: -6.58788 LUMO: 1.83133 factor:1 | 1 (-0.75389) | -1 | -1 |
| G: -5345.34143 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11610.22452 HOMO: -7.08584 LUMO: 1.91568 factor:1 | 1 (-0.51740) | 1 | 1 |
| G: -5345.34143 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11609.97997 HOMO: -6.56883 LUMO: 1.81228 factor:1 | 1 (-0.27285) | -1 | -1 |
| G: -5345.34143 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11610.09211 HOMO: -6.66135 LUMO: 1.92384 factor:1 | 1 (-0.38499) | -1 | -1 |
| G: -5345.34143 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11609.92218 HOMO: -6.64502 LUMO: 2.15786 factor:1 | 1 (-0.21505) | -1 | -1 |
| G: -5345.34143 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11610.24069 HOMO: -6.71305 LUMO: 1.91840 factor:1 | 1 (-0.53356) | -1 | -1 |
| G: -5345.34143 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11610.17103 HOMO: -6.44094 LUMO: 1.74425 factor:1 | 1 (-0.46390) | -1 | -1 |
| G: -5345.34143 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11610.09023 HOMO: -6.51985 LUMO: 1.84221 factor:1 | 1 (-0.38311) | -1 | -1 |
| G: -5345.34143 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11609.96008 HOMO: -6.63414 LUMO: -0.24762 factor:1 | 1 (-0.25296) | -1 | -1 |
| G: -5345.34143 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11609.82209 HOMO: -6.60420 LUMO: -0.22585 factor:1 | 1 (-0.11497) | -1 | -1 |
| G: -5345.34143 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11609.70702 HOMO: -7.19741 LUMO: 0.58232 factor:1 | -1 (0.00011) | -1 | -1 |
| G: -5345.34143 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11609.87921 HOMO: -6.77019 LUMO: -0.56872 factor:1 | 1 (-0.17208) | -1 | -1 |
| G: -5345.34143 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11609.93298 HOMO: -7.46136 LUMO: 0.28844 factor:1 | 1 (-0.22585) | -1 | -1 |
| G: -5345.34143 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11609.87023 HOMO: -6.60420 LUMO: -0.54151 factor:1 | 1 (-0.16311) | -1 | -1 |
| G: -5345.34143 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11609.72898 HOMO: -6.53890 LUMO: -0.46531 factor:1 | 1 (-0.02185) | -1 | -1 |
| G: -5345.34143 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11610.15573 HOMO: -6.81645 LUMO: -0.57144 factor:1 | 1 (-0.44861) | -1 | -1 |
| G: -5345.34143 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11610.09238 HOMO: -7.48041 LUMO: 0.28572 factor:1 | 1 (-0.38526) | -1 | -1 |
| G: -5345.34143 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11610.06384 HOMO: -6.75659 LUMO: -0.45715 factor:1 | 1 (-0.35671) | -1 | -1 |
| G: -5345.34143 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11609.86680 HOMO: -6.66135 LUMO: -0.41906 factor:1 | 1 (-0.15968) | -1 | -1 |
| G: -5345.34143 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11610.32458 HOMO: -6.55794 LUMO: -0.27483 factor:1 | 1 (-0.61745) | -1 | -1 |
| G: -5345.34143 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11610.14493 HOMO: -7.07496 LUMO: -0.63403 factor:1 | 1 (-0.43780) | -1 | -1 |
| G: -5345.34143 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11610.16504 HOMO: -7.12394 LUMO: 0.53334 factor:1 | 1 (-0.45791) | -1 | -1 |
| G: -5345.34143 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11610.16931 HOMO: -6.53617 LUMO: -0.25579 factor:1 | 1 (-0.46219) | -1 | -1 |
| G: -5345.34143 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11610.43917 HOMO: -6.50896 LUMO: -0.25034 factor:1 | 1 (-0.73204) | -1 | -1 |
| G: -5345.34143 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11610.32082 HOMO: -7.17564 LUMO: -0.68573 factor:1 | 1 (-0.61370) | -1 | -1 |
| G: -5345.34143 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11610.04438 HOMO: -6.53617 LUMO: -0.30749 factor:1 | 1 (-0.33726) | -1 | -1 |
| G: -5345.34143 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11609.90727 HOMO: -6.55522 LUMO: -0.30749 factor:1 | 1 (-0.20014) | -1 | -1 |
| G: -5345.34143 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11609.92781 HOMO: -7.05591 LUMO: -0.71022 factor:1 | 1 (-0.22068) | -1 | -1 |
| G: -5345.34143 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11610.15992 HOMO: -7.17564 LUMO: -0.69933 factor:1 | 1 (-0.45280) | -1 | -1 |
| G: -5345.34143 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11609.91513 HOMO: -6.78380 LUMO: -0.67756 factor:1 | 1 (-0.20800) | -1 | -1 |
| G: -5345.34143 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11610.14077 HOMO: -6.62325 LUMO: 2.02725 factor:1 | 1 (-0.43364) | -1 | -1 |
| G: -5345.34143 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11610.01617 HOMO: -6.63414 LUMO: 1.91296 factor:1 | 1 (-0.30904) | -1 | -1 |
| G: -5345.34143 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11610.23979 HOMO: -6.83278 LUMO: 1.65717 factor:1 | 1 (-0.53266) | -1 | -1 |
| G: -5345.34143 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11610.21674 HOMO: -6.66407 LUMO: 1.95650 factor:1 | 1 (-0.50961) | -1 | -1 |
| G: -5345.34143 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11610.17590 HOMO: -6.61237 LUMO: 2.11432 factor:1 | 1 (-0.46877) | -1 | -1 |
| G: -5345.34143 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11610.38063 HOMO: -6.62053 LUMO: 2.09256 factor:1 | 1 (-0.67351) | -1 | -1 |
| G: -5345.34143 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11610.05679 HOMO: -6.78652 LUMO: 2.13609 factor:1 | 1 (-0.34967) | -1 | -1 |
| G: -5345.34143 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11609.99641 HOMO: -6.94707 LUMO: 1.81772 factor:1 | 1 (-0.28928) | -1 | -1 |
| G: -5345.34143 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11610.32379 HOMO: -6.85183 LUMO: 2.12793 factor:1 | 1 (-0.61666) | -1 | -1 |
| G: -5345.34143 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11609.86724 HOMO: -6.81101 LUMO: 1.83949 factor:1 | 1 (-0.16011) | -1 | -1 |
| G: -5345.34143 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11609.79698 HOMO: -6.98788 LUMO: 2.16058 factor:1 | 1 (-0.08985) | -1 | -1 |
| G: -5345.34143 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11609.71689 HOMO: -6.62869 LUMO: 2.00820 factor:1 | 1 (-0.00977) | -1 | -1 |
| G: -5345.34143 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11610.23720 HOMO: -6.34025 LUMO: 2.25855 factor:1 | 1 (-0.53008) | -1 | -1 |
| G: -5345.34143 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11610.20458 HOMO: -6.01372 LUMO: 2.01636 factor:1 | 1 (-0.49745) | -1 | -1 |
| G: -5345.34143 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11610.18972 HOMO: -6.89264 LUMO: 2.27487 factor:1 | 1 (-0.48259) | -1 | -1 |
| G: -5345.34143 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11610.39903 HOMO: -6.53073 LUMO: 2.20684 factor:1 | 1 (-0.69190) | -1 | -1 |
| G: -5345.34143 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11610.04860 HOMO: -6.83278 LUMO: 1.53744 factor:1 | 1 (-0.34148) | -1 | -1 |
| G: -5345.34143 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11610.04817 HOMO: -6.41917 LUMO: 1.82316 factor:1 | 1 (-0.34104) | -1 | -1 |
| G: -5345.34143 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11609.97418 HOMO: -6.56339 LUMO: 1.63813 factor:1 | 1 (-0.26705) | -1 | -1 |
| G: -5345.34143 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11610.01423 HOMO: -6.88992 LUMO: 1.65173 factor:1 | 1 (-0.30711) | -1 | -1 |
| G: -5345.34143 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11609.88128 HOMO: -6.63141 LUMO: 1.92112 factor:1 | 1 (-0.17415) | -1 | -1 |
| G: -5345.34143 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11610.08267 HOMO: -6.83822 LUMO: 1.88847 factor:1 | 1 (-0.37554) | -1 | -1 |
| G: -5345.34143 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11609.95831 HOMO: -6.84638 LUMO: 1.90480 factor:1 | 1 (-0.25119) | -1 | -1 |
| G: -5345.34143 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11610.14996 HOMO: -6.82462 LUMO: 1.70888 factor:1 | 1 (-0.44284) | -1 | -1 |
| G: -5345.34143 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11610.12879 HOMO: -6.82734 LUMO: 2.12521 factor:1 | 1 (-0.42167) | -1 | -1 |
| G: -5345.34143 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11610.20569 HOMO: -6.94435 LUMO: 1.87214 factor:1 | 1 (-0.49857) | -1 | -1 |
| G: -5345.34143 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11610.16332 HOMO: -6.98516 LUMO: 2.51433 factor:1 | 1 (-0.45620) | -1 | -1 |
| G: -5345.34143 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11609.87333 HOMO: -6.74026 LUMO: 2.15514 factor:1 | 1 (-0.16621) | -1 | -1 |
| G: -5345.34143 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11609.82492 HOMO: -6.93618 LUMO: 2.54426 factor:1 | 1 (-0.11780) | -1 | -1 |
| G: -5345.34143 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11609.70122 HOMO: -6.28583 LUMO: 2.53610 factor:1 | -1 (0.00590) | -1 | -1 |
| G: -5345.34143 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11609.95222 HOMO: -6.56883 LUMO: 1.94834 factor:1 | 1 (-0.24509) | -1 | -1 |
| G: -5345.34143 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11609.81992 HOMO: -7.08584 LUMO: 1.99187 factor:1 | 1 (-0.11279) | 1 | 1 |
| G: -5345.34143 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11609.63292 HOMO: -6.19059 LUMO: 1.99732 factor:1 | -1 (0.07421) | -1 | -1 |
| G: -5345.34143 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11609.90495 HOMO: -6.78108 LUMO: 2.03813 factor:1 | 1 (-0.19783) | -1 | -1 |
| G: -5345.34143 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11610.01562 HOMO: -6.82189 LUMO: 1.77418 factor:1 | 1 (-0.30850) | -1 | -1 |
| G: -5345.34143 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11609.96452 HOMO: -6.45454 LUMO: 1.78779 factor:1 | 1 (-0.25739) | -1 | -1 |
| G: -5345.34143 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11610.18221 HOMO: -6.84366 LUMO: 1.77690 factor:1 | 1 (-0.47508) | -1 | -1 |
| G: -5345.34143 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11609.75333 HOMO: -6.74026 LUMO: 1.67622 factor:1 | 1 (-0.04620) | -1 | -1 |
| G: -5345.34143 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11610.00743 HOMO: -6.76475 LUMO: 2.40277 factor:1 | 1 (-0.30030) | -1 | -1 |
| G: -5345.34143 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11609.90416 HOMO: -6.65863 LUMO: 1.86670 factor:1 | 1 (-0.19704) | -1 | -1 |
| G: -5345.34143 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11610.03804 HOMO: -6.50080 LUMO: 1.93201 factor:1 | 1 (-0.33092) | -1 | -1 |
| G: -5345.34143 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11610.16414 HOMO: -6.34842 LUMO: 1.70888 factor:1 | 1 (-0.45702) | -1 | -1 |
| G: -5345.34143 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11610.24741 HOMO: -6.60692 LUMO: 2.20140 factor:1 | 1 (-0.54028) | -1 | -1 |
| G: -5345.34143 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11610.05489 HOMO: -6.74026 LUMO: 2.14970 factor:1 | 1 (-0.34776) | -1 | -1 |
| G: -5345.34143 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11610.37337 HOMO: -6.63686 LUMO: 2.17419 factor:1 | 1 (-0.66624) | -1 | -1 |
| G: -5345.34143 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11610.13470 HOMO: -6.81917 LUMO: 2.10072 factor:1 | 1 (-0.42757) | -1 | -1 |
| G: -5345.34143 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11610.05238 HOMO: -6.92802 LUMO: 2.04358 factor:1 | 1 (-0.34526) | -1 | -1 |
| G: -5345.34143 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11609.93488 HOMO: -6.56067 LUMO: -0.47620 factor:1 | 1 (-0.22776) | -1 | -1 |
| G: -5345.34143 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11610.31906 HOMO: -6.56611 LUMO: -0.77008 factor:1 | 1 (-0.61193) | -1 | -1 |
| G: -5345.34143 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11609.92688 HOMO: -6.78380 LUMO: -0.64763 factor:1 | 1 (-0.21976) | -1 | -1 |
| G: -5345.34143 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11609.84351 HOMO: -6.51985 LUMO: -0.24490 factor:1 | 1 (-0.13638) | -1 | -1 |
| G: -5345.34143 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11609.73877 HOMO: -6.52529 LUMO: -0.27483 factor:1 | 1 (-0.03165) | -1 | -1 |
| G: -5345.34143 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11610.13905 HOMO: -7.10489 LUMO: -0.62586 factor:1 | 1 (-0.43193) | -1 | -1 |
| G: -5345.34143 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11610.19685 HOMO: -7.18108 LUMO: 0.48980 factor:1 | 1 (-0.48972) | -1 | -1 |
| G: -5345.34143 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11610.16787 HOMO: -7.14299 LUMO: -0.63947 factor:1 | 1 (-0.46074) | -1 | -1 |
| G: -5345.34143 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11610.46178 HOMO: -6.70761 LUMO: -0.54423 factor:1 | 1 (-0.75465) | -1 | -1 |
| G: -5345.34143 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11610.25873 HOMO: -7.32258 LUMO: -1.03675 factor:1 | 1 (-0.55160) | -1 | -1 |
| G: -5345.34143 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11610.17415 HOMO: -6.65046 LUMO: -0.41361 factor:1 | 1 (-0.46703) | -1 | -1 |
| G: -5345.34143 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11610.14071 HOMO: -6.76475 LUMO: -0.60137 factor:1 | 1 (-0.43359) | -1 | -1 |
| G: -5345.34143 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11609.95148 HOMO: -6.77836 LUMO: -0.54423 factor:1 | 1 (-0.24436) | -1 | -1 |
| G: -5345.34143 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11610.01083 HOMO: -7.52395 LUMO: 0.26395 factor:1 | 1 (-0.30371) | -1 | -1 |
| G: -5345.34143 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11610.00787 HOMO: -6.93890 LUMO: -0.72382 factor:1 | 1 (-0.30074) | -1 | -1 |
| G: -5345.34143 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11610.19168 HOMO: -6.72938 LUMO: -0.47348 factor:1 | 1 (-0.48455) | -1 | -1 |
| G: -5345.34143 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11610.23791 HOMO: -6.66951 LUMO: -0.40817 factor:1 | 1 (-0.53079) | -1 | -1 |
| G: -5345.34143 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11610.04798 HOMO: -6.60420 LUMO: -0.19320 factor:1 | 1 (-0.34085) | -1 | -1 |
| G: -5345.34143 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11610.17467 HOMO: -6.67495 LUMO: -0.27211 factor:1 | 1 (-0.46755) | -1 | -1 |
| G: -5345.34143 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11610.24763 HOMO: -7.23823 LUMO: -0.62858 factor:1 | 1 (-0.54050) | -1 | -1 |
| G: -5345.34143 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11610.02925 HOMO: -7.27088 LUMO: 0.53334 factor:1 | 1 (-0.32213) | -1 | -1 |
| G: -5345.34143 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11610.13630 HOMO: -7.20013 LUMO: 0.59049 factor:1 | 1 (-0.42918) | -1 | -1 |
| G: -5345.34143 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11609.90547 HOMO: -6.60148 LUMO: -0.20953 factor:1 | 1 (-0.19834) | -1 | -1 |
| G: -5345.34143 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11610.12403 HOMO: -6.69400 LUMO: -0.51974 factor:1 | 1 (-0.41691) | -1 | -1 |
| G: -5345.34143 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11609.92683 HOMO: -7.40422 LUMO: -0.98777 factor:1 | 1 (-0.21970) | -1 | -1 |
| G: -5345.34143 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11610.01540 HOMO: -6.88176 LUMO: -0.71022 factor:1 | 1 (-0.30828) | -1 | -1 |
| G: -5345.34143 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11609.85159 HOMO: -6.86271 LUMO: -0.59321 factor:1 | 1 (-0.14447) | -1 | -1 |
| G: -5345.34143 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11610.04866 HOMO: -6.73754 LUMO: -0.55239 factor:1 | 1 (-0.34153) | -1 | -1 |
| G: -5345.34143 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11609.86686 HOMO: -6.71033 LUMO: 1.57010 factor:1 | 1 (-0.15973) | -1 | -1 |
| G: -5345.34143 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11609.81072 HOMO: -6.69672 LUMO: 1.68711 factor:1 | 1 (-0.10359) | -1 | -1 |
| G: -5345.34143 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11609.66941 HOMO: -6.67495 LUMO: 2.03813 factor:1 | -1 (0.03771) | -1 | -1 |
| G: -5345.34143 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11610.12479 HOMO: -6.54434 LUMO: 1.83677 factor:1 | 1 (-0.41767) | -1 | -1 |
| G: -5345.34143 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11609.92645 HOMO: -6.57155 LUMO: 1.77146 factor:1 | 1 (-0.21932) | -1 | -1 |
| G: -5345.34143 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11609.71687 HOMO: -6.76747 LUMO: 1.87759 factor:1 | 1 (-0.00974) | -1 | -1 |
| G: -5345.34143 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11610.02000 HOMO: -6.58243 LUMO: 1.61364 factor:1 | 1 (-0.31288) | -1 | -1 |
| G: -5345.34143 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11609.82326 HOMO: -6.61781 LUMO: 2.13881 factor:1 | 1 (-0.11614) | -1 | -1 |
| G: -5345.34143 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11610.18474 HOMO: -6.62597 LUMO: 2.00276 factor:1 | 1 (-0.47761) | -1 | -1 |
| G: -5345.34143 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11610.02425 HOMO: -7.01237 LUMO: 1.95922 factor:1 | 1 (-0.31712) | -1 | -1 |
| G: -5345.34143 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11610.18354 HOMO: -7.03959 LUMO: 2.16875 factor:1 | 1 (-0.47642) | -1 | -1 |
| G: -5345.34143 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11610.11456 HOMO: -6.83278 LUMO: 1.91296 factor:1 | 1 (-0.40744) | -1 | -1 |
| G: -5345.34143 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11609.73349 HOMO: -6.40012 LUMO: 1.95650 factor:1 | 1 (-0.02637) | -1 | -1 |
| G: -5345.34143 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11610.14166 HOMO: -6.50080 LUMO: 1.73337 factor:1 | 1 (-0.43454) | -1 | -1 |
| G: -5345.34143 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11610.09179 HOMO: -6.95795 LUMO: 2.28848 factor:1 | 1 (-0.38466) | -1 | -1 |
| G: -5345.34143 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11610.30305 HOMO: -6.63686 LUMO: 2.20140 factor:1 | 1 (-0.59593) | -1 | -1 |
| G: -5345.34143 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11610.37024 HOMO: -6.57427 LUMO: 1.87214 factor:1 | 1 (-0.66311) | -1 | -1 |
| G: -5345.34143 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11610.25579 HOMO: -6.38379 LUMO: 2.32113 factor:1 | 1 (-0.54866) | -1 | -1 |
| G: -5345.34143 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11610.10471 HOMO: -6.63958 LUMO: 2.04902 factor:1 | 1 (-0.39759) | -1 | -1 |
| G: -5345.34143 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11609.88337 HOMO: -6.70216 LUMO: 1.93201 factor:1 | 1 (-0.17625) | -1 | -1 |
| G: -5345.34143 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11610.08047 HOMO: -6.80557 LUMO: 2.23678 factor:1 | 1 (-0.37334) | -1 | -1 |
| G: -5345.34143 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11610.08572 HOMO: -6.72938 LUMO: 2.28304 factor:1 | 1 (-0.37859) | -1 | -1 |
| G: -5345.34143 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11610.09391 HOMO: -6.56067 LUMO: 1.66806 factor:1 | 1 (-0.38678) | -1 | -1 |
| G: -5345.34143 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11609.88343 HOMO: -6.95523 LUMO: 2.33474 factor:1 | 1 (-0.17630) | -1 | -1 |
| G: -5345.34143 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11610.24303 HOMO: -6.59876 LUMO: 2.30480 factor:1 | 1 (-0.53590) | -1 | -1 |
| G: -5345.34143 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11610.03940 HOMO: -6.87360 LUMO: 1.75786 factor:1 | 1 (-0.33228) | -1 | -1 |
| G: -5345.34143 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11610.32017 HOMO: -7.06408 LUMO: 1.99187 factor:1 | 1 (-0.61305) | 1 | 1 |
| G: -5345.34143 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11610.17837 HOMO: -6.95795 LUMO: 1.88847 factor:1 | 1 (-0.47125) | -1 | -1 |
| G: -5345.34143 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11610.04196 HOMO: -6.85455 LUMO: 1.63813 factor:1 | 1 (-0.33484) | -1 | -1 |
| G: -5345.34143 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11609.90405 HOMO: -7.09129 LUMO: 2.31569 factor:1 | 1 (-0.19693) | 1 | 1 |
| G: -5345.34143 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11610.17426 HOMO: -6.91441 LUMO: 1.68983 factor:1 | 1 (-0.46714) | -1 | -1 |
| G: -5345.34143 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11610.02716 HOMO: -6.89809 LUMO: 2.23678 factor:1 | 1 (-0.32003) | -1 | -1 |
| G: -5345.34143 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11609.93080 HOMO: -6.78652 LUMO: 1.98371 factor:1 | 1 (-0.22368) | -1 | -1 |
| G: -5345.34143 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11610.19622 HOMO: -6.94707 LUMO: 2.23678 factor:1 | 1 (-0.48910) | -1 | -1 |
| G: -5345.34143 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11609.97954 HOMO: -7.07224 LUMO: 2.13337 factor:1 | 1 (-0.27241) | 1 | 1 |
| G: -5345.34143 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11609.87916 HOMO: -6.94979 LUMO: 2.28031 factor:1 | 1 (-0.17203) | -1 | -1 |
| G: -5345.34143 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11609.78416 HOMO: -6.60965 LUMO: 2.20412 factor:1 | 1 (-0.07704) | -1 | -1 |
| G: -5345.34143 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11610.08776 HOMO: -6.87360 LUMO: 2.40277 factor:1 | 1 (-0.38063) | -1 | -1 |
| G: -5345.34143 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11610.04112 HOMO: -6.92802 LUMO: 1.89663 factor:1 | 1 (-0.33399) | -1 | -1 |
| G: -5345.34143 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11610.12063 HOMO: -6.88448 LUMO: 2.02725 factor:1 | 1 (-0.41350) | -1 | -1 |
| G: -5345.34143 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11610.24077 HOMO: -6.69128 LUMO: 1.55105 factor:1 | 1 (-0.53364) | -1 | -1 |
| G: -5345.34143 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11610.16909 HOMO: -6.54978 LUMO: 1.93201 factor:1 | 1 (-0.46197) | -1 | -1 |
| G: -5345.34143 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11610.18188 HOMO: -6.19331 LUMO: 1.46941 factor:1 | 1 (-0.47476) | -1 | -1 |
| G: -5345.34143 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11610.18934 HOMO: -6.55794 LUMO: 1.89663 factor:1 | 1 (-0.48221) | -1 | -1 |
| G: -5345.34143 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11610.03078 HOMO: -6.07630 LUMO: 1.94289 factor:1 | 1 (-0.32365) | -1 | -1 |
| G: -5345.34143 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11610.04847 HOMO: -7.46408 LUMO: 0.31565 factor:1 | 1 (-0.34134) | -1 | -1 |
| G: -5345.34143 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11609.89839 HOMO: -6.63958 LUMO: -0.61770 factor:1 | 1 (-0.19127) | -1 | -1 |
| G: -5345.34143 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11609.82857 HOMO: -6.81101 LUMO: -0.57960 factor:1 | 1 (-0.12144) | -1 | -1 |
| G: -5345.34143 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11610.09902 HOMO: -6.74298 LUMO: -0.57960 factor:1 | 1 (-0.39190) | -1 | -1 |
| G: -5345.34143 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11609.99665 HOMO: -6.63686 LUMO: -0.42994 factor:1 | 1 (-0.28953) | -1 | -1 |
| G: -5345.34143 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11609.78813 HOMO: -6.60965 LUMO: -0.41089 factor:1 | 1 (-0.08101) | -1 | -1 |
| G: -5345.34143 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11610.02357 HOMO: -6.60692 LUMO: -0.80274 factor:1 | 1 (-0.31644) | -1 | -1 |
| G: -5345.34143 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11609.80661 HOMO: -6.58788 LUMO: -0.78097 factor:1 | 1 (-0.09948) | -1 | -1 |
| G: -5345.34143 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11609.93714 HOMO: -6.67767 LUMO: -0.48436 factor:1 | 1 (-0.23002) | -1 | -1 |
| G: -5345.34143 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11610.02183 HOMO: -6.63141 LUMO: -0.40545 factor:1 | 1 (-0.31470) | -1 | -1 |
| G: -5345.34143 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11609.83499 HOMO: -6.62053 LUMO: -0.83811 factor:1 | 1 (-0.12787) | -1 | -1 |
| G: -5345.34143 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11609.96229 HOMO: -6.59604 LUMO: -0.35375 factor:1 | 1 (-0.25516) | -1 | -1 |
| G: -5345.34143 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11609.87624 HOMO: -6.34297 LUMO: -0.39729 factor:1 | 1 (-0.16912) | -1 | -1 |
| G: -5345.34143 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11609.68196 HOMO: -6.67223 LUMO: 1.97827 factor:1 | -1 (0.02517) | -1 | -1 |
| G: -5345.34143 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11610.06613 HOMO: -6.40012 LUMO: 1.89935 factor:1 | 1 (-0.35900) | -1 | -1 |
| G: -5345.30015 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11610.46015 HOMO: -6.74842 LUMO: 1.97283 factor:1 | 1 (-0.79430) | -1 | -1 |
| G: -5345.30015 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11610.39288 HOMO: -6.76747 LUMO: 2.17147 factor:1 | 1 (-0.72703) | -1 | -1 |
| G: -5345.30015 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11610.19614 HOMO: -6.72121 LUMO: 1.55649 factor:1 | 1 (-0.53030) | -1 | -1 |
| G: -5345.30015 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11610.32518 HOMO: -6.97700 LUMO: 2.04085 factor:1 | 1 (-0.65933) | -1 | -1 |
| G: -5345.30015 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11610.40232 HOMO: -7.06680 LUMO: 2.04085 factor:1 | 1 (-0.73648) | 1 | 1 |
| G: -5345.30015 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11610.22809 HOMO: -7.09673 LUMO: 2.35106 factor:1 | 1 (-0.56224) | 1 | 1 |
| G: -5345.30015 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11610.44472 HOMO: -6.83006 LUMO: 2.14970 factor:1 | 1 (-0.77887) | -1 | -1 |
| G: -5345.30015 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11610.33541 HOMO: -6.72665 LUMO: 2.20140 factor:1 | 1 (-0.66956) | -1 | -1 |
| G: -5345.30015 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11610.33829 HOMO: -6.77291 LUMO: 2.34562 factor:1 | 1 (-0.67245) | -1 | -1 |
| G: -5345.30015 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11610.46793 HOMO: -6.73754 LUMO: 2.00276 factor:1 | 1 (-0.80208) | -1 | -1 |
| G: -5345.30015 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11610.37819 HOMO: -7.04231 LUMO: 1.92112 factor:1 | 1 (-0.71234) | -1 | -1 |
| G: -5345.30015 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11610.48050 HOMO: -6.83822 LUMO: 1.72248 factor:1 | 1 (-0.81465) | -1 | -1 |
| G: -5345.30015 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11610.27761 HOMO: -6.57971 LUMO: 2.16603 factor:1 | 1 (-0.61177) | -1 | -1 |
| G: -5345.30015 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11610.20224 HOMO: -6.80013 LUMO: 1.88575 factor:1 | 1 (-0.53639) | -1 | -1 |
| G: -5345.30015 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11610.41351 HOMO: -6.93618 LUMO: 2.18235 factor:1 | 1 (-0.74766) | -1 | -1 |
| G: -5345.30015 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11610.28352 HOMO: -6.54706 LUMO: 1.91024 factor:1 | 1 (-0.61767) | -1 | -1 |
| G: -5345.30015 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11610.03230 HOMO: -7.06952 LUMO: 2.18507 factor:1 | 1 (-0.36646) | 1 | 1 |
| G: -5345.30015 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11610.15867 HOMO: -7.05047 LUMO: 1.82044 factor:1 | 1 (-0.49283) | -1 | -1 |
| G: -5345.30015 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11610.03559 HOMO: -6.87632 LUMO: 1.92657 factor:1 | 1 (-0.36975) | -1 | -1 |
| G: -5345.30015 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11610.19018 HOMO: -6.58788 LUMO: 1.91568 factor:1 | 1 (-0.52434) | -1 | -1 |
| G: -5345.30015 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11610.08047 HOMO: -7.17292 LUMO: 1.90752 factor:1 | 1 (-0.41462) | 1 | 1 |
| G: -5345.30015 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11610.34978 HOMO: -6.93890 LUMO: 1.80684 factor:1 | 1 (-0.68393) | -1 | -1 |
| G: -5345.30015 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11610.16871 HOMO: -7.10761 LUMO: 2.20956 factor:1 | 1 (-0.50287) | 1 | 1 |
| G: -5345.30015 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11610.32183 HOMO: -6.85727 LUMO: 2.13609 factor:1 | 1 (-0.65598) | -1 | -1 |
| G: -5345.30015 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11610.19024 HOMO: -6.64502 LUMO: 1.38506 factor:1 | 1 (-0.52439) | -1 | -1 |
| G: -5345.30015 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11610.14953 HOMO: -6.87360 LUMO: 1.15648 factor:1 | 1 (-0.48368) | -1 | -1 |
| G: -5345.30015 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11610.49574 HOMO: -6.67223 LUMO: 2.07351 factor:1 | 1 (-0.82989) | -1 | -1 |
| G: -5345.30015 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11610.19609 HOMO: -6.29671 LUMO: 2.43270 factor:1 | 1 (-0.53024) | -1 | -1 |
| G: -5345.30015 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11609.86596 HOMO: -6.90897 LUMO: 2.28848 factor:1 | 1 (-0.20011) | -1 | -1 |
| G: -5345.30015 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11610.05053 HOMO: -7.04231 LUMO: 1.70071 factor:1 | 1 (-0.38469) | -1 | -1 |
| G: -5345.30015 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11610.08131 HOMO: -6.69944 LUMO: 1.94834 factor:1 | 1 (-0.41546) | -1 | -1 |
| G: -5345.30015 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11610.29005 HOMO: -6.56067 LUMO: 2.20956 factor:1 | 1 (-0.62420) | -1 | -1 |
| G: -5345.30015 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11610.14599 HOMO: -6.65046 LUMO: 2.06807 factor:1 | 1 (-0.48014) | -1 | -1 |
| G: -5345.30015 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11609.92182 HOMO: -7.08584 LUMO: 1.98915 factor:1 | 1 (-0.25598) | 1 | 1 |
| G: -5345.30015 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11609.89121 HOMO: -6.69400 LUMO: 2.09256 factor:1 | 1 (-0.22536) | -1 | -1 |
| G: -5345.30015 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11610.11658 HOMO: -6.62869 LUMO: 2.16331 factor:1 | 1 (-0.45073) | -1 | -1 |
| G: -5345.30015 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11610.17854 HOMO: -6.85183 LUMO: 2.16058 factor:1 | 1 (-0.51269) | -1 | -1 |
| G: -5345.30015 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11610.09864 HOMO: -6.54706 LUMO: 1.92384 factor:1 | 1 (-0.43280) | -1 | -1 |
| G: -5345.30015 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11610.25282 HOMO: -6.84366 LUMO: 2.48984 factor:1 | 1 (-0.58698) | -1 | -1 |
| G: -5345.30015 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11610.17445 HOMO: -6.77291 LUMO: 2.46263 factor:1 | 1 (-0.50861) | -1 | -1 |
| G: -5345.30015 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11610.06705 HOMO: -7.01782 LUMO: 2.31025 factor:1 | 1 (-0.40120) | -1 | -1 |
| G: -5345.30015 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11610.38050 HOMO: -6.94707 LUMO: 2.29664 factor:1 | 1 (-0.71465) | -1 | -1 |
| G: -5345.30015 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11609.81532 HOMO: -6.64230 LUMO: 1.97283 factor:1 | 1 (-0.14947) | -1 | -1 |
| G: -5345.30015 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11609.86971 HOMO: -6.47359 LUMO: 2.20412 factor:1 | 1 (-0.20387) | -1 | -1 |
| G: -5345.30015 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11609.82174 HOMO: -6.90625 LUMO: 1.92384 factor:1 | 1 (-0.15589) | -1 | -1 |
| G: -5345.30015 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11610.17728 HOMO: -7.17020 LUMO: 2.06807 factor:1 | 1 (-0.51144) | 1 | 1 |
| G: -5345.30015 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11610.16615 HOMO: -6.65046 LUMO: 2.20956 factor:1 | 1 (-0.50031) | -1 | -1 |
| G: -5345.30015 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11610.11524 HOMO: -7.07496 LUMO: 1.82861 factor:1 | 1 (-0.44940) | 1 | 1 |
| G: -5345.30015 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11610.37451 HOMO: -6.83006 LUMO: 2.14970 factor:1 | 1 (-0.70867) | -1 | -1 |
| G: -5345.30015 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11610.28776 HOMO: -6.92802 LUMO: 1.99187 factor:1 | 1 (-0.62192) | -1 | -1 |
| G: -5345.30015 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11610.34627 HOMO: -6.69672 LUMO: 2.36739 factor:1 | 1 (-0.68042) | -1 | -1 |
| G: -5345.30015 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11610.01929 HOMO: -7.13755 LUMO: 2.00276 factor:1 | 1 (-0.35345) | 1 | 1 |
| G: -5345.30015 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11610.14224 HOMO: -6.92530 LUMO: 2.25582 factor:1 | 1 (-0.47639) | -1 | -1 |
| G: -5345.30015 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11610.01021 HOMO: -6.77564 LUMO: 1.97827 factor:1 | 1 (-0.34436) | -1 | -1 |
| G: -5345.30015 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11609.87540 HOMO: -6.87904 LUMO: 1.60003 factor:1 | 1 (-0.20955) | -1 | -1 |
| G: -5345.30015 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11610.16009 HOMO: -6.62869 LUMO: 1.90480 factor:1 | 1 (-0.49424) | -1 | -1 |
| G: -5345.30015 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11609.95641 HOMO: -6.71033 LUMO: 1.54833 factor:1 | 1 (-0.29056) | -1 | -1 |
| G: -5345.30015 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11609.97616 HOMO: -6.74298 LUMO: 1.47486 factor:1 | 1 (-0.31032) | -1 | -1 |
| G: -5345.30015 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11610.11252 HOMO: -6.77019 LUMO: 1.90480 factor:1 | 1 (-0.44667) | -1 | -1 |
| G: -5345.30015 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11610.11723 HOMO: -6.70489 LUMO: 1.99459 factor:1 | 1 (-0.45138) | -1 | -1 |