乙二醇作为反应物的反应表19-19

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: -5278.76361 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.82499 HOMO: -6.91169 LUMO: -0.53879 factor:1 | 1 (-0.69569) | -1 | -1 |
| G: -5278.76361 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.61285 HOMO: -7.29809 LUMO: 2.83543 factor:1 | 1 (-0.48355) | 1 | -1 |
| G: -5278.76361 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.60343 HOMO: -6.86543 LUMO: -0.70205 factor:1 | 1 (-0.47413) | -1 | -1 |
| G: -5278.76361 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.64229 HOMO: -7.47769 LUMO: 0.31293 factor:1 | 1 (-0.51299) | -1 | -1 |
| G: -5278.76361 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.79644 HOMO: -6.63141 LUMO: -0.55511 factor:1 | 1 (-0.66714) | -1 | -1 |
| G: -5278.76361 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.60764 HOMO: -6.68856 LUMO: -0.30205 factor:1 | 1 (-1.47834) | -1 | -1 |
| G: -5278.76361 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.62473 HOMO: -7.22190 LUMO: 0.53334 factor:1 | 1 (-1.49543) | -1 | -1 |
| G: -5278.76361 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.69776 HOMO: -6.66407 LUMO: -0.27756 factor:1 | 1 (-1.56846) | -1 | -1 |
| G: -5278.76361 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.47281 HOMO: -7.15659 LUMO: -0.70205 factor:1 | 1 (-1.34351) | -1 | -1 |
| G: -5278.76361 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.97581 HOMO: -6.69400 LUMO: 1.67622 factor:1 | 1 (-1.84651) | -1 | -1 |
| G: -5278.76361 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.91692 HOMO: -6.60420 LUMO: 2.16058 factor:1 | 1 (-1.78762) | -1 | -1 |
| G: -5278.76361 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11545.71405 HOMO: -6.87087 LUMO: 1.88031 factor:1 | 1 (-2.58476) | -1 | -1 |
| G: -5278.76361 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11546.31907 HOMO: -6.60965 LUMO: -0.19864 factor:1 | 1 (-3.18977) | -1 | -1 |
| G: -5278.76361 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11545.59484 HOMO: -7.29265 LUMO: 0.52246 factor:1 | 1 (-2.46554) | -1 | -1 |
| G: -5278.76361 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11545.79876 HOMO: -6.86543 LUMO: -0.59593 factor:1 | 1 (-2.66946) | -1 | -1 |
| G: -5278.76361 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11545.44891 HOMO: -7.44504 LUMO: -1.01226 factor:1 | 1 (-2.31961) | -1 | -1 |
| G: -5278.76361 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.66582 HOMO: -6.92530 LUMO: -0.75103 factor:1 | 1 (-1.53652) | -1 | -1 |
| G: -5278.76361 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.80906 HOMO: -7.10489 LUMO: 2.20412 factor:1 | 1 (-1.67976) | 1 | 1 |
| G: -5278.76361 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.52935 HOMO: -6.58788 LUMO: 1.73881 factor:1 | 1 (-1.40005) | -1 | -1 |
| G: -5278.76361 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.57001 HOMO: -6.64502 LUMO: 1.70343 factor:1 | 1 (-1.44071) | -1 | -1 |
| G: -5278.76361 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.42043 HOMO: -6.73754 LUMO: 1.60819 factor:1 | 1 (-1.29113) | -1 | -1 |
| G: -5278.76361 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.21575 HOMO: -6.80829 LUMO: 2.45991 factor:1 | 1 (-0.08645) | -1 | -1 |
| G: -5278.76361 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.37665 HOMO: -6.91713 LUMO: 2.43814 factor:1 | 1 (-0.24735) | -1 | -1 |
| G: -5278.76361 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.42669 HOMO: -6.60692 LUMO: 1.93745 factor:1 | 1 (-0.29739) | -1 | -1 |
| G: -5278.76361 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.11150 HOMO: -6.26134 LUMO: 1.46125 factor:1 | -1 (0.01780) | -1 | -1 |
| G: -5278.76361 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.31896 HOMO: -7.54028 LUMO: 0.25851 factor:1 | 1 (-0.18966) | -1 | -1 |
| G: -5278.76361 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.86896 HOMO: -6.97700 LUMO: -0.73471 factor:1 | 1 (-0.73966) | -1 | -1 |
| G: -5278.76361 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.60536 HOMO: -6.92258 LUMO: -0.70205 factor:1 | 1 (-0.47606) | -1 | -1 |
| G: -5278.76361 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.69500 HOMO: -6.83550 LUMO: -0.56872 factor:1 | 1 (-0.56570) | -1 | -1 |
| G: -5278.76361 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.81644 HOMO: -6.72121 LUMO: 1.89663 factor:1 | 1 (-0.68714) | -1 | -1 |
| G: -5278.76361 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.64142 HOMO: -6.73482 LUMO: 1.89935 factor:1 | 1 (-0.51212) | -1 | -1 |
| G: -5278.76361 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.47034 HOMO: -6.61781 LUMO: 1.86670 factor:1 | 1 (-0.34104) | -1 | -1 |
| G: -5278.76361 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11542.83651 HOMO: -7.01782 LUMO: 2.26399 factor:1 | -1 (0.29279) | -1 | -1 |
| G: -5278.76361 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11542.98927 HOMO: -7.23551 LUMO: 2.09800 factor:1 | -1 (0.14003) | 1 | 1 |
| G: -5278.76361 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11542.82230 HOMO: -7.13483 LUMO: 2.17963 factor:1 | -1 (0.30700) | 1 | 1 |
| G: -5278.76361 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.53192 HOMO: -6.22869 LUMO: 2.01092 factor:1 | 1 (-0.40262) | -1 | -1 |
| G: -5278.76361 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.64215 HOMO: -6.80285 LUMO: 2.14970 factor:1 | 1 (-0.51285) | -1 | -1 |
| G: -5278.76361 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.79143 HOMO: -7.21102 LUMO: 2.33746 factor:1 | 1 (-0.66213) | 1 | 1 |
| G: -5278.76361 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.51480 HOMO: -6.39740 LUMO: 2.59597 factor:1 | 1 (-0.38550) | -1 | -1 |
| G: -5278.76361 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.52879 HOMO: -7.07768 LUMO: 2.48168 factor:1 | 1 (-0.39949) | 1 | 1 |
| G: -5278.76361 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.82997 HOMO: -7.11306 LUMO: 0.90614 factor:1 | 1 (-0.70067) | -1 | -1 |
| G: -5278.76361 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.56180 HOMO: -6.61781 LUMO: -2.46263 factor:1 | 1 (-0.43250) | -1 | -1 |
| G: -5278.76361 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.59989 HOMO: -6.96611 LUMO: 0.90614 factor:1 | 1 (-0.47059) | -1 | -1 |
| G: -5278.76361 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.76752 HOMO: -6.86271 LUMO: -1.14832 factor:1 | 1 (-0.63822) | -1 | -1 |
| G: -5278.76361 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.48835 HOMO: -6.72665 LUMO: 0.96873 factor:1 | 1 (-0.35905) | -1 | -1 |
| G: -5278.76361 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.42122 HOMO: -7.14571 LUMO: 1.05036 factor:1 | 1 (-0.29192) | -1 | -1 |
| G: -5278.76361 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.68545 HOMO: -7.14299 LUMO: 0.98777 factor:1 | 1 (-0.55615) | -1 | -1 |
| G: -5278.76361 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.61374 HOMO: -6.99333 LUMO: 1.05852 factor:1 | 1 (-0.48444) | -1 | -1 |
| G: -5278.76361 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.73821 HOMO: -6.78924 LUMO: -1.49935 factor:1 | 1 (-0.60891) | -1 | -1 |
| G: -5278.76361 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.44158 HOMO: -7.13755 LUMO: 0.94151 factor:1 | 1 (-0.31228) | -1 | -1 |
| G: -5278.76361 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.52876 HOMO: -6.72938 LUMO: -0.35375 factor:1 | 1 (-0.39946) | -1 | -1 |
| G: -5278.76361 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.60387 HOMO: -6.99061 LUMO: 0.82450 factor:1 | 1 (-0.47457) | -1 | -1 |
| G: -5278.76361 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.68743 HOMO: -6.75114 LUMO: -0.68028 factor:1 | 1 (-0.55813) | -1 | -1 |
| G: -5278.76361 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.37450 HOMO: -6.40556 LUMO: -0.42722 factor:1 | 1 (-0.24520) | -1 | -1 |
| G: -5278.76361 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.71625 HOMO: -7.18653 LUMO: 0.42178 factor:1 | 1 (-0.58695) | -1 | -1 |
| G: -5278.76361 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.61502 HOMO: -6.63958 LUMO: -0.71294 factor:1 | 1 (-0.48572) | -1 | -1 |
| G: -5278.76361 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.53303 HOMO: -6.63958 LUMO: -0.71022 factor:1 | 1 (-0.40374) | -1 | -1 |
| G: -5278.76361 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.79829 HOMO: -6.69672 LUMO: -0.72654 factor:1 | 1 (-0.66899) | -1 | -1 |
| G: -5278.76361 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.54879 HOMO: -6.56883 LUMO: -0.80274 factor:1 | 1 (-0.41949) | -1 | -1 |
| G: -5278.76361 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.53989 HOMO: -6.68584 LUMO: -0.56872 factor:1 | 1 (-0.41059) | -1 | -1 |
| G: -5278.76361 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.69309 HOMO: -6.59060 LUMO: -0.35647 factor:1 | 1 (-0.56379) | -1 | -1 |
| G: -5278.76361 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.36900 HOMO: -6.72121 LUMO: -0.71838 factor:1 | 1 (-0.23971) | -1 | -1 |
| G: -5278.76361 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.32124 HOMO: -6.57971 LUMO: -0.61498 factor:1 | 1 (-1.19194) | -1 | -1 |
| G: -5278.76361 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.41351 HOMO: -7.07496 LUMO: 0.50613 factor:1 | 1 (-1.28421) | -1 | -1 |
| G: -5278.76361 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.11277 HOMO: -7.14027 LUMO: 0.43266 factor:1 | 1 (-0.98347) | -1 | -1 |
| G: -5278.76361 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.32021 HOMO: -6.43277 LUMO: -0.44082 factor:1 | 1 (-1.19091) | -1 | -1 |
| G: -5278.76361 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.33270 HOMO: -6.79468 LUMO: 0.07619 factor:1 | 1 (-1.20340) | -1 | -1 |
| G: -5278.76361 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.97530 HOMO: -6.81917 LUMO: -2.57148 factor:1 | 1 (-0.84600) | -1 | -1 |
| G: -5278.76361 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.15999 HOMO: -6.71849 LUMO: 1.30615 factor:1 | 1 (-1.03069) | -1 | -1 |
| G: -5278.76361 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.05593 HOMO: -6.85455 LUMO: -0.63675 factor:1 | 1 (-0.92663) | -1 | -1 |
| G: -5278.76361 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.80537 HOMO: -6.73210 LUMO: -1.03131 factor:1 | 1 (-0.67607) | -1 | -1 |
| G: -5278.76361 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.18741 HOMO: -6.83550 LUMO: -0.58777 factor:1 | 1 (-1.05811) | -1 | -1 |
| G: -5278.76361 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.37502 HOMO: -6.53073 LUMO: -0.74287 factor:1 | 1 (-0.24572) | -1 | -1 |
| G: -5278.76361 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.36745 HOMO: -7.18381 LUMO: -0.92791 factor:1 | 1 (-0.23815) | -1 | -1 |
| G: -5278.76361 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.20399 HOMO: -6.49264 LUMO: -0.44627 factor:1 | 1 (-0.07470) | -1 | -1 |
| G: -5278.76361 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.30713 HOMO: -7.32803 LUMO: 0.41361 factor:1 | 1 (-0.17783) | -1 | -1 |
| G: -5278.76361 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.20639 HOMO: -6.53073 LUMO: -0.52790 factor:1 | 1 (-0.07709) | -1 | -1 |
| G: -5278.76361 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.32454 HOMO: -6.54978 LUMO: -0.53062 factor:1 | 1 (-0.19524) | -1 | -1 |
| G: -5278.76361 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.36405 HOMO: -6.56611 LUMO: -0.37824 factor:1 | 1 (-0.23475) | -1 | -1 |
| G: -5278.76361 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.11534 HOMO: -6.57155 LUMO: -0.64219 factor:1 | -1 (0.01396) | -1 | -1 |
| G: -5278.76361 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.16794 HOMO: -7.08040 LUMO: 0.45715 factor:1 | 1 (-0.03864) | -1 | -1 |
| G: -5278.76361 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11542.90151 HOMO: -6.66679 LUMO: -0.75376 factor:1 | -1 (0.22779) | -1 | -1 |
| G: -5278.76361 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.31504 HOMO: -6.83550 LUMO: -0.99322 factor:1 | 1 (-0.18574) | -1 | -1 |
| G: -5278.76361 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.12622 HOMO: -6.53345 LUMO: -0.29660 factor:1 | -1 (0.00307) | -1 | -1 |
| G: -5278.76361 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.14514 HOMO: -6.65046 LUMO: 2.40549 factor:1 | 1 (-0.01584) | -1 | -1 |
| G: -5278.76361 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.12114 HOMO: -6.98788 LUMO: 2.01092 factor:1 | -1 (0.00816) | -1 | -1 |
| G: -5278.76361 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11542.72020 HOMO: -6.61781 LUMO: 1.92384 factor:1 | -1 (0.40910) | -1 | -1 |
| G: -5278.76361 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.12023 HOMO: -6.61237 LUMO: 2.06807 factor:1 | 1 (-0.99093) | -1 | -1 |
| G: -5278.76361 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.02978 HOMO: -6.59060 LUMO: 1.95106 factor:1 | 1 (-0.90048) | -1 | -1 |
| G: -5278.76361 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.23425 HOMO: -6.48175 LUMO: 1.72248 factor:1 | 1 (-1.10495) | -1 | -1 |
| G: -5278.76361 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.03310 HOMO: -6.84911 LUMO: 2.03541 factor:1 | 1 (-0.90380) | -1 | -1 |
| G: -5278.76361 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.83533 HOMO: -6.50624 LUMO: 2.17147 factor:1 | 1 (-0.70603) | -1 | -1 |
| G: -5278.76361 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.93089 HOMO: -6.68312 LUMO: 2.08439 factor:1 | 1 (-0.80159) | -1 | -1 |
| G: -5278.76361 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.17710 HOMO: -6.96067 LUMO: 1.98099 factor:1 | 1 (-1.04780) | -1 | -1 |
| G: -5278.76361 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.20644 HOMO: -6.93618 LUMO: 1.85854 factor:1 | 1 (-1.07714) | -1 | -1 |
| G: -5278.76361 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.21278 HOMO: -6.71305 LUMO: -0.61226 factor:1 | 1 (-1.08348) | -1 | -1 |
| G: -5278.76361 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11542.89515 HOMO: -7.06408 LUMO: 0.80001 factor:1 | -1 (0.23415) | -1 | -1 |
| G: -5278.76361 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11542.69999 HOMO: -6.52257 LUMO: 0.99049 factor:1 | -1 (0.42931) | -1 | -1 |
| G: -5278.76361 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11542.83683 HOMO: -6.84638 LUMO: 1.10750 factor:1 | -1 (0.29247) | -1 | -1 |
| G: -5278.76361 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11542.93196 HOMO: -6.85455 LUMO: 0.84900 factor:1 | -1 (0.19734) | -1 | -1 |
| G: -5278.76361 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11542.85936 HOMO: -6.60148 LUMO: -0.78369 factor:1 | -1 (0.26994) | -1 | -1 |
| G: -5278.76361 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11542.91847 HOMO: -6.86543 LUMO: -0.93063 factor:1 | -1 (0.21083) | -1 | -1 |
| G: -5278.76361 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11542.89593 HOMO: -6.70489 LUMO: -0.72382 factor:1 | -1 (0.23336) | -1 | -1 |
| G: -5278.76361 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.00240 HOMO: -6.59060 LUMO: 0.31293 factor:1 | 1 (-0.87310) | -1 | -1 |
| G: -5278.76361 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.89759 HOMO: -6.52257 LUMO: -0.48708 factor:1 | 1 (-0.76829) | -1 | -1 |
| G: -5278.76361 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.05653 HOMO: -6.54706 LUMO: -0.48164 factor:1 | 1 (-0.92723) | -1 | -1 |
| G: -5278.76361 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.91750 HOMO: -7.32803 LUMO: 0.08436 factor:1 | 1 (-0.78821) | -1 | -1 |
| G: -5278.76361 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.78202 HOMO: -6.77291 LUMO: -0.66940 factor:1 | 1 (-0.65272) | -1 | -1 |
| G: -5278.76361 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.94390 HOMO: -6.68312 LUMO: -0.53062 factor:1 | 1 (-0.81460) | -1 | -1 |
| G: -5278.76361 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.05261 HOMO: -7.07768 LUMO: 0.45987 factor:1 | 1 (-0.92331) | -1 | -1 |
| G: -5278.76361 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11542.38202 HOMO: -6.50352 LUMO: -0.63675 factor:1 | -1 (0.74728) | -1 | -1 |
| G: -5278.76361 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11542.90013 HOMO: -6.48992 LUMO: -0.60681 factor:1 | -1 (0.22917) | -1 | -1 |
| G: -5278.76361 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.00598 HOMO: -6.65318 LUMO: -0.72382 factor:1 | -1 (0.12332) | -1 | -1 |
| G: -5278.76361 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11542.88108 HOMO: -6.54706 LUMO: 0.24218 factor:1 | -1 (0.24822) | -1 | -1 |
| G: -5278.76361 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11542.38988 HOMO: -6.63958 LUMO: 0.57416 factor:1 | -1 (0.73941) | -1 | -1 |
| G: -5278.76361 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11542.55647 HOMO: -6.37563 LUMO: -0.48164 factor:1 | -1 (0.57283) | -1 | -1 |
| G: -5278.76361 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11542.54951 HOMO: -6.64774 LUMO: -0.71838 factor:1 | -1 (0.57979) | -1 | -1 |
| G: -5278.76361 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11542.67471 HOMO: -7.17020 LUMO: 0.45987 factor:1 | -1 (0.45459) | -1 | -1 |
| G: -5278.76361 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11542.67735 HOMO: -6.86543 LUMO: -1.05036 factor:1 | -1 (0.45195) | -1 | -1 |
| G: -5278.76361 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11542.69286 HOMO: -6.77019 LUMO: -1.03131 factor:1 | -1 (0.43644) | -1 | -1 |
| G: -5278.76361 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.13544 HOMO: -6.80285 LUMO: 1.05852 factor:1 | 1 (-1.00614) | -1 | -1 |
| G: -5278.76361 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.17188 HOMO: -6.76475 LUMO: 1.01771 factor:1 | 1 (-1.04258) | -1 | -1 |
| G: -5278.76361 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.97013 HOMO: -6.92530 LUMO: 1.37417 factor:1 | 1 (-0.84083) | -1 | -1 |
| G: -5278.76361 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.92447 HOMO: -6.98244 LUMO: 1.25989 factor:1 | 1 (-0.79517) | -1 | -1 |
| G: -5278.76361 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.21381 HOMO: -6.74842 LUMO: 0.89798 factor:1 | 1 (-1.08451) | -1 | -1 |
| G: -5278.76361 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.09114 HOMO: -6.77019 LUMO: -1.17009 factor:1 | 1 (-0.96184) | -1 | -1 |
| G: -5278.76361 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.01925 HOMO: -6.78652 LUMO: 1.35785 factor:1 | 1 (-0.88995) | -1 | -1 |
| G: -5278.76361 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.22181 HOMO: -6.82734 LUMO: -0.68301 factor:1 | 1 (-1.09251) | -1 | -1 |
| G: -5278.76361 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.84289 HOMO: -6.48175 LUMO: -2.19052 factor:1 | 1 (-0.71359) | -1 | -1 |
| G: -5278.76361 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.64153 HOMO: -6.65863 LUMO: -0.77008 factor:1 | 1 (-0.51223) | -1 | -1 |
| G: -5278.76361 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.80950 HOMO: -6.44094 LUMO: -2.20956 factor:1 | 1 (-0.68020) | -1 | -1 |
| G: -5278.76361 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.83413 HOMO: -6.59876 LUMO: -0.57688 factor:1 | 1 (-0.70483) | -1 | -1 |
| G: -5278.76361 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.00991 HOMO: -6.78380 LUMO: -0.77008 factor:1 | 1 (-0.88061) | -1 | -1 |
| G: -5278.76361 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.74444 HOMO: -7.30354 LUMO: 0.25034 factor:1 | 1 (-0.61514) | -1 | -1 |
| G: -5278.76361 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.56865 HOMO: -6.59332 LUMO: -0.53334 factor:1 | 1 (-0.43936) | -1 | -1 |
| G: -5278.76361 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.61211 HOMO: -6.64230 LUMO: -0.55783 factor:1 | 1 (-0.48281) | -1 | -1 |
| G: -5278.76361 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.60120 HOMO: -7.26544 LUMO: 0.20409 factor:1 | 1 (-0.47190) | -1 | -1 |
| G: -5278.76361 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.69742 HOMO: -6.61237 LUMO: -0.65307 factor:1 | 1 (-0.56812) | -1 | -1 |
| G: -5278.76361 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.77062 HOMO: -6.72393 LUMO: -0.65307 factor:1 | 1 (-0.64132) | -1 | -1 |
| G: -5278.76361 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.60928 HOMO: -6.29671 LUMO: -0.39729 factor:1 | 1 (-0.47998) | -1 | -1 |
| G: -5278.76361 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.44419 HOMO: -6.75387 LUMO: -0.53334 factor:1 | 1 (-0.31489) | -1 | -1 |
| G: -5278.76361 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.49374 HOMO: -6.53073 LUMO: -0.31293 factor:1 | 1 (-0.36444) | -1 | -1 |
| G: -5278.76361 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.35368 HOMO: -6.42189 LUMO: -0.59049 factor:1 | 1 (-0.22439) | -1 | -1 |
| G: -5278.76361 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.37034 HOMO: -6.41100 LUMO: -0.29933 factor:1 | 1 (-0.24104) | -1 | -1 |
| G: -5278.76361 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.25221 HOMO: -6.57427 LUMO: -0.53879 factor:1 | 1 (-0.12291) | -1 | -1 |
| G: -5278.76361 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.39086 HOMO: -7.43143 LUMO: 0.33470 factor:1 | 1 (-0.26156) | -1 | -1 |
| G: -5278.76361 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.30124 HOMO: -6.56067 LUMO: -0.50885 factor:1 | 1 (-1.17194) | -1 | -1 |
| G: -5278.76361 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.16758 HOMO: -6.65863 LUMO: -0.76464 factor:1 | 1 (-1.03828) | -1 | -1 |
| G: -5278.76361 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.72155 HOMO: -6.32665 LUMO: -0.41906 factor:1 | 1 (-1.59225) | -1 | -1 |
| G: -5278.76361 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.33963 HOMO: -6.57699 LUMO: 1.63813 factor:1 | 1 (-1.21034) | -1 | -1 |
| G: -5278.76361 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.04368 HOMO: -6.53073 LUMO: 1.71704 factor:1 | 1 (-0.91438) | -1 | -1 |
| G: -5278.76361 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.23865 HOMO: -6.86271 LUMO: 2.07351 factor:1 | 1 (-1.10935) | -1 | -1 |
| G: -5278.76361 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.49512 HOMO: -6.63686 LUMO: 1.78235 factor:1 | 1 (-1.36582) | -1 | -1 |
| G: -5278.76361 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.11585 HOMO: -6.60965 LUMO: 1.94289 factor:1 | 1 (-0.98655) | -1 | -1 |
| G: -5278.76361 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.37038 HOMO: -6.55250 LUMO: 1.89119 factor:1 | 1 (-1.24108) | -1 | -1 |
| G: -5278.76361 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.19427 HOMO: -6.50624 LUMO: 1.85582 factor:1 | 1 (-1.06497) | -1 | -1 |
| G: -5278.76361 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.15677 HOMO: -6.06814 LUMO: 1.94561 factor:1 | 1 (-1.02747) | -1 | -1 |
| G: -5278.76361 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.14624 HOMO: -6.58788 LUMO: 2.01908 factor:1 | 1 (-1.01694) | -1 | -1 |
| G: -5278.76361 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.96439 HOMO: -6.74026 LUMO: 0.31293 factor:1 | 1 (-0.83509) | -1 | -1 |
| G: -5278.76361 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.45751 HOMO: -6.54434 LUMO: -0.42994 factor:1 | 1 (-1.32821) | -1 | -1 |
| G: -5278.76361 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.40688 HOMO: -6.94707 LUMO: 0.42994 factor:1 | 1 (-0.27758) | -1 | -1 |
| G: -5278.76361 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.18168 HOMO: -6.98516 LUMO: 0.41361 factor:1 | 1 (-0.05238) | -1 | -1 |
| G: -5278.76361 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.50688 HOMO: -6.31304 LUMO: -0.54967 factor:1 | 1 (-0.37759) | -1 | -1 |
| G: -5278.76361 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.26144 HOMO: -6.48447 LUMO: -0.40817 factor:1 | 1 (-0.13214) | -1 | -1 |
| G: -5278.76361 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.45409 HOMO: -6.49264 LUMO: 0.29116 factor:1 | 1 (-0.32480) | -1 | -1 |
| G: -5278.76361 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.37363 HOMO: -6.48719 LUMO: -0.11973 factor:1 | 1 (-0.24433) | -1 | -1 |
| G: -5278.76361 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.14046 HOMO: -7.16204 LUMO: 0.44082 factor:1 | 1 (-0.01116) | -1 | -1 |
| G: -5278.76361 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.34775 HOMO: -6.74842 LUMO: -0.37552 factor:1 | 1 (-0.21845) | -1 | -1 |
| G: -5278.76361 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.41567 HOMO: -6.44638 LUMO: -0.45171 factor:1 | 1 (-0.28637) | -1 | -1 |
| G: -5278.76361 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.21575 HOMO: -7.07496 LUMO: 0.50341 factor:1 | 1 (-0.08645) | -1 | -1 |
| G: -5278.76361 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.59108 HOMO: -6.79468 LUMO: 0.11429 factor:1 | 1 (-0.46178) | -1 | -1 |
| G: -5278.76361 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.82371 HOMO: -6.63958 LUMO: -0.67484 factor:1 | 1 (-0.69441) | -1 | -1 |
| G: -5278.76361 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.94485 HOMO: -7.08584 LUMO: 0.46259 factor:1 | 1 (-0.81555) | -1 | -1 |
| G: -5278.76361 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.03538 HOMO: -6.80285 LUMO: -0.73199 factor:1 | 1 (-0.90608) | -1 | -1 |
| G: -5278.76361 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.74322 HOMO: -6.44366 LUMO: -0.45443 factor:1 | 1 (-0.61392) | -1 | -1 |
| G: -5278.76361 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.98991 HOMO: -6.75931 LUMO: 0.25851 factor:1 | 1 (-0.86061) | -1 | -1 |
| G: -5278.76361 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.74631 HOMO: -6.64502 LUMO: 1.79323 factor:1 | 1 (-1.61701) | -1 | -1 |
| G: -5278.76361 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.97695 HOMO: -6.51168 LUMO: 1.60275 factor:1 | 1 (-1.84765) | -1 | -1 |
| G: -5278.76361 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.67025 HOMO: -6.56067 LUMO: 1.63268 factor:1 | 1 (-1.54095) | -1 | -1 |
| G: -5278.76361 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.76892 HOMO: -6.56883 LUMO: 1.70615 factor:1 | 1 (-1.63962) | -1 | -1 |
| G: -5278.76361 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.27484 HOMO: -6.77836 LUMO: 1.77962 factor:1 | 1 (-1.14554) | -1 | -1 |
| G: -5278.76361 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.35953 HOMO: -6.38923 LUMO: 1.85854 factor:1 | 1 (-1.23023) | -1 | -1 |
| G: -5278.76361 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.37991 HOMO: -6.35658 LUMO: 2.16875 factor:1 | 1 (-1.25061) | -1 | -1 |
| G: -5278.76361 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.38742 HOMO: -6.83006 LUMO: 2.31025 factor:1 | 1 (-1.25812) | -1 | -1 |
| G: -5278.76361 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.28448 HOMO: -6.87087 LUMO: 1.79051 factor:1 | 1 (-1.15518) | -1 | -1 |
| G: -5278.76361 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.36508 HOMO: -6.56339 LUMO: 2.37828 factor:1 | 1 (-1.23578) | -1 | -1 |
| G: -5278.76361 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.26872 HOMO: -6.30488 LUMO: 2.51705 factor:1 | 1 (-1.13942) | -1 | -1 |
| G: -5278.76361 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.11182 HOMO: -6.69400 LUMO: 1.95650 factor:1 | 1 (-0.98252) | -1 | -1 |
| G: -5278.76361 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.11680 HOMO: -6.51168 LUMO: 2.03541 factor:1 | 1 (-0.98750) | -1 | -1 |
| G: -5278.76361 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.05998 HOMO: -6.30760 LUMO: 1.65173 factor:1 | 1 (-0.93068) | -1 | -1 |
| G: -5278.76361 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.39392 HOMO: -6.55250 LUMO: 1.90752 factor:1 | 1 (-1.26462) | -1 | -1 |
| G: -5278.76361 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.31212 HOMO: -6.41372 LUMO: 1.76058 factor:1 | 1 (-1.18282) | -1 | -1 |
| G: -5278.76361 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.96790 HOMO: -6.23957 LUMO: 2.06534 factor:1 | 1 (-0.83860) | -1 | -1 |
| G: -5278.76361 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.89612 HOMO: -6.58243 LUMO: 2.11705 factor:1 | 1 (-0.76682) | -1 | -1 |
| G: -5278.76361 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.96262 HOMO: -6.37835 LUMO: 2.09256 factor:1 | 1 (-0.83332) | -1 | -1 |
| G: -5278.76361 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.04202 HOMO: -6.50624 LUMO: 2.55787 factor:1 | 1 (-0.91272) | -1 | -1 |
| G: -5278.76361 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.19321 HOMO: -6.45454 LUMO: 1.87214 factor:1 | 1 (-1.06391) | -1 | -1 |
| G: -5278.76361 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11545.00191 HOMO: -6.53617 LUMO: 1.95650 factor:1 | 1 (-1.87261) | -1 | -1 |
| G: -5278.76361 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.91839 HOMO: -6.51985 LUMO: 1.71432 factor:1 | 1 (-1.78909) | -1 | -1 |
| G: -5278.76361 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.75387 HOMO: -6.75114 LUMO: 1.84493 factor:1 | 1 (-1.62457) | -1 | -1 |
| G: -5278.76361 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.77458 HOMO: -6.06270 LUMO: 1.65717 factor:1 | 1 (-1.64528) | -1 | -1 |
| G: -5278.76361 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.99056 HOMO: -5.89671 LUMO: 1.71704 factor:1 | 1 (-1.86126) | -1 | -1 |
| G: -5278.76361 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.71278 HOMO: -6.18787 LUMO: 1.91840 factor:1 | 1 (-1.58348) | -1 | -1 |
| G: -5278.76361 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.67227 HOMO: -6.01644 LUMO: 1.85582 factor:1 | 1 (-1.54297) | -1 | -1 |
| G: -5278.76361 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.81823 HOMO: -6.05998 LUMO: 2.33474 factor:1 | 1 (-1.68893) | -1 | -1 |
| G: -5278.76361 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.71444 HOMO: -6.05725 LUMO: 2.03541 factor:1 | 1 (-1.58514) | -1 | -1 |
| G: -5278.76361 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.74223 HOMO: -6.80829 LUMO: 1.90480 factor:1 | 1 (-1.61293) | -1 | -1 |
| G: -5278.76361 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.83809 HOMO: -6.76475 LUMO: 2.20956 factor:1 | 1 (-1.70879) | -1 | -1 |
| G: -5278.76361 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.54688 HOMO: -6.29944 LUMO: 1.77962 factor:1 | 1 (-1.41758) | -1 | -1 |
| G: -5278.76361 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.93812 HOMO: -6.47359 LUMO: -0.25579 factor:1 | 1 (-1.80882) | -1 | -1 |
| G: -5278.76361 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11545.00479 HOMO: -6.57699 LUMO: -0.47348 factor:1 | 1 (-1.87549) | -1 | -1 |
| G: -5278.76361 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11545.17347 HOMO: -7.20830 LUMO: 0.49797 factor:1 | 1 (-2.04417) | -1 | -1 |
| G: -5278.76361 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11546.02179 HOMO: -7.49402 LUMO: 0.29933 factor:1 | 1 (-2.89249) | -1 | -1 |
| G: -5278.76361 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.91235 HOMO: -6.66679 LUMO: -0.58777 factor:1 | 1 (-1.78305) | -1 | -1 |
| G: -5278.76361 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.87641 HOMO: -6.67767 LUMO: -0.56328 factor:1 | 1 (-1.74711) | -1 | -1 |
| G: -5278.76361 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.95320 HOMO: -7.42871 LUMO: 0.35647 factor:1 | 1 (-1.82390) | -1 | -1 |
| G: -5278.76361 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11545.00514 HOMO: -6.56067 LUMO: -0.54423 factor:1 | 1 (-1.87584) | -1 | -1 |
| G: -5278.76361 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.73779 HOMO: -6.56339 LUMO: -0.50341 factor:1 | 1 (-1.60849) | -1 | -1 |
| G: -5278.76361 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11545.94821 HOMO: -6.56067 LUMO: -0.48436 factor:1 | 1 (-2.81891) | -1 | -1 |
| G: -5278.76361 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11545.61506 HOMO: -6.73210 LUMO: 1.75241 factor:1 | 1 (-2.48576) | -1 | -1 |
| G: -5278.76361 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11545.79534 HOMO: -6.48175 LUMO: 1.91296 factor:1 | 1 (-2.66604) | -1 | -1 |
| G: -5278.76361 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11546.44620 HOMO: -6.67767 LUMO: 1.70343 factor:1 | 1 (-3.31690) | -1 | -1 |
| G: -5278.76361 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11546.46147 HOMO: -6.37835 LUMO: 1.96466 factor:1 | 1 (-3.33217) | -1 | -1 |
| G: -5278.76361 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11545.49647 HOMO: -6.40828 LUMO: 2.10072 factor:1 | 1 (-2.36717) | -1 | -1 |
| G: -5278.76361 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11545.15432 HOMO: -6.06542 LUMO: 1.92112 factor:1 | 1 (-2.02502) | -1 | -1 |
| G: -5278.76361 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11545.22890 HOMO: -6.90353 LUMO: 1.83133 factor:1 | 1 (-2.09960) | -1 | -1 |
| G: -5278.76361 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11545.29075 HOMO: -6.37019 LUMO: 1.92929 factor:1 | 1 (-2.16145) | -1 | -1 |
| G: -5278.76361 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.82718 HOMO: -6.61509 LUMO: 2.11160 factor:1 | 1 (-1.69788) | -1 | -1 |
| G: -5278.76361 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11545.03872 HOMO: -6.82734 LUMO: 1.77146 factor:1 | 1 (-1.90942) | -1 | -1 |
| G: -5278.76361 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.93505 HOMO: -6.01100 LUMO: 1.89935 factor:1 | 1 (-1.80575) | -1 | -1 |
| G: -5278.76361 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.72598 HOMO: -6.49536 LUMO: 1.75241 factor:1 | 1 (-1.59668) | -1 | -1 |
| G: -5278.76361 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11545.02509 HOMO: -6.34297 LUMO: 1.86398 factor:1 | 1 (-1.89579) | -1 | -1 |
| G: -5278.76361 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.70299 HOMO: -6.53073 LUMO: 1.84493 factor:1 | 1 (-1.57369) | -1 | -1 |
| G: -5278.76361 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.94631 HOMO: -6.53345 LUMO: 2.41093 factor:1 | 1 (-1.81701) | -1 | -1 |
| G: -5278.76361 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11545.00022 HOMO: -7.01237 LUMO: 2.06262 factor:1 | 1 (-1.87092) | -1 | -1 |
| G: -5278.76361 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.60443 HOMO: -6.17154 LUMO: 1.89119 factor:1 | 1 (-1.47513) | -1 | -1 |
| G: -5278.76361 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11545.14221 HOMO: -6.08719 LUMO: 1.74425 factor:1 | 1 (-2.01291) | -1 | -1 |
| G: -5278.76361 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.90245 HOMO: -6.69672 LUMO: 1.95106 factor:1 | 1 (-1.77315) | -1 | -1 |
| G: -5278.76361 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11545.74785 HOMO: -6.58243 LUMO: 2.24766 factor:1 | 1 (-2.61855) | -1 | -1 |
| G: -5278.76361 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11545.75490 HOMO: -6.74570 LUMO: 2.02181 factor:1 | 1 (-2.62560) | -1 | -1 |
| G: -5278.76361 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11546.58438 HOMO: -6.53890 LUMO: 1.92929 factor:1 | 1 (-3.45508) | -1 | -1 |
| G: -5278.76361 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11545.80997 HOMO: -6.03276 LUMO: 1.67078 factor:1 | 1 (-2.68068) | -1 | -1 |
| G: -5278.76361 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11545.57370 HOMO: -6.67767 LUMO: 2.03541 factor:1 | 1 (-2.44440) | -1 | -1 |
| G: -5278.76361 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11545.04577 HOMO: -5.98378 LUMO: 1.84221 factor:1 | 1 (-1.91647) | -1 | -1 |
| G: -5278.76361 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11545.12210 HOMO: -6.07086 LUMO: 2.01908 factor:1 | 1 (-1.99280) | -1 | -1 |
| G: -5278.76361 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.89012 HOMO: -6.29944 LUMO: 1.90208 factor:1 | 1 (-1.76082) | -1 | -1 |
| G: -5278.76361 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11545.10898 HOMO: -6.75114 LUMO: 1.85854 factor:1 | 1 (-1.97968) | -1 | -1 |
| G: -5278.76361 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.77233 HOMO: -6.56611 LUMO: 2.49801 factor:1 | 1 (-0.64303) | -1 | -1 |
| G: -5278.76361 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.84104 HOMO: -6.39740 LUMO: 1.92929 factor:1 | 1 (-0.71174) | -1 | -1 |
| G: -5278.76361 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.88107 HOMO: -6.85999 LUMO: -1.07757 factor:1 | 1 (-0.75177) | -1 | -1 |
| G: -5278.76361 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.92480 HOMO: -6.98244 LUMO: 1.07213 factor:1 | 1 (-0.79550) | -1 | -1 |
| G: -5278.76361 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.65508 HOMO: -7.04231 LUMO: 0.64219 factor:1 | 1 (-0.52578) | -1 | -1 |
| G: -5278.76361 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.66561 HOMO: -6.96339 LUMO: 0.75648 factor:1 | 1 (-0.53631) | -1 | -1 |
| G: -5278.76361 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.76088 HOMO: -6.83822 LUMO: -0.97417 factor:1 | 1 (-0.63158) | -1 | -1 |
| G: -5278.76361 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.54171 HOMO: -6.44910 LUMO: -2.15242 factor:1 | 1 (-1.41241) | -1 | -1 |
| G: -5278.76361 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.65406 HOMO: -6.84094 LUMO: -1.37690 factor:1 | 1 (-1.52476) | -1 | -1 |
| G: -5278.76361 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.75651 HOMO: -6.74026 LUMO: -2.54699 factor:1 | 1 (-1.62721) | -1 | -1 |
| G: -5278.76361 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.46122 HOMO: -6.96611 LUMO: 1.24900 factor:1 | 1 (-1.33192) | -1 | -1 |
| G: -5278.76361 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.55218 HOMO: -7.21102 LUMO: 0.82995 factor:1 | 1 (-1.42288) | -1 | -1 |
| G: -5278.76361 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.60397 HOMO: -6.88448 LUMO: 0.81634 factor:1 | 1 (-1.47467) | -1 | -1 |
| G: -5278.76361 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.62726 HOMO: -7.04231 LUMO: 1.10750 factor:1 | 1 (-1.49796) | -1 | -1 |
| G: -5278.76361 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.63725 HOMO: -6.83550 LUMO: -0.98777 factor:1 | 1 (-1.50795) | -1 | -1 |
| G: -5278.76361 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.32072 HOMO: -6.82189 LUMO: 0.93879 factor:1 | 1 (-1.19142) | -1 | -1 |
| G: -5278.76361 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.25558 HOMO: -6.81101 LUMO: 0.70750 factor:1 | 1 (-1.12628) | -1 | -1 |
| G: -5278.76361 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.55273 HOMO: -7.06680 LUMO: 0.74015 factor:1 | 1 (-1.42343) | -1 | -1 |
| G: -5278.76361 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.42633 HOMO: -6.68856 LUMO: 0.86260 factor:1 | 1 (-1.29703) | -1 | -1 |
| G: -5278.76361 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11545.01829 HOMO: -6.83822 LUMO: -0.63403 factor:1 | 1 (-1.88899) | -1 | -1 |
| G: -5278.76361 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11545.12096 HOMO: -6.84911 LUMO: 1.26533 factor:1 | 1 (-1.99166) | -1 | -1 |
| G: -5278.76361 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.83271 HOMO: -7.01237 LUMO: 0.73743 factor:1 | 1 (-1.70341) | -1 | -1 |
| G: -5278.76361 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11545.13636 HOMO: -7.00965 LUMO: 1.40139 factor:1 | 1 (-2.00706) | -1 | -1 |
| G: -5278.76361 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11545.84970 HOMO: -6.73210 LUMO: -2.49256 factor:1 | 1 (-2.72040) | -1 | -1 |
| G: -5278.76361 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11546.48112 HOMO: -7.08040 LUMO: 0.84627 factor:1 | 1 (-3.35182) | -1 | -1 |
| G: -5278.76361 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11545.78312 HOMO: -7.00965 LUMO: 0.82995 factor:1 | 1 (-2.65382) | -1 | -1 |
| G: -5278.76361 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11545.75308 HOMO: -6.88448 LUMO: 0.82723 factor:1 | 1 (-2.62378) | -1 | -1 |
| G: -5278.76361 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11545.46953 HOMO: -7.20013 LUMO: 0.88437 factor:1 | 1 (-2.34023) | -1 | -1 |
| G: -5278.76361 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.99045 HOMO: -6.60420 LUMO: -0.53334 factor:1 | 1 (-1.86115) | -1 | -1 |
| G: -5278.76361 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.73700 HOMO: -6.78652 LUMO: -0.79729 factor:1 | 1 (-1.60770) | -1 | -1 |
| G: -5278.76361 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.88593 HOMO: -6.48992 LUMO: -0.64491 factor:1 | 1 (-1.75663) | -1 | -1 |
| G: -5278.76361 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.95693 HOMO: -6.85999 LUMO: -0.78097 factor:1 | 1 (-1.82763) | -1 | -1 |
| G: -5278.76361 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.99630 HOMO: -6.65046 LUMO: -0.78097 factor:1 | 1 (-1.86700) | -1 | -1 |
| G: -5278.76361 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11545.12395 HOMO: -7.24095 LUMO: 0.37280 factor:1 | 1 (-1.99465) | -1 | -1 |
| G: -5278.76361 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.84190 HOMO: -6.81101 LUMO: -0.74831 factor:1 | 1 (-1.71260) | -1 | -1 |
| G: -5278.76361 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.81816 HOMO: -6.69400 LUMO: -0.77280 factor:1 | 1 (-0.68886) | -1 | -1 |
| G: -5278.76361 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.46220 HOMO: -6.08447 LUMO: -0.68573 factor:1 | 1 (-0.33290) | -1 | -1 |
| G: -5278.76361 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.58218 HOMO: -6.66679 LUMO: -0.47076 factor:1 | 1 (-0.45288) | -1 | -1 |
| G: -5278.76361 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.81652 HOMO: -6.97428 LUMO: -1.10750 factor:1 | 1 (-0.68722) | -1 | -1 |
| G: -5278.76361 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.51401 HOMO: -6.69128 LUMO: -0.54151 factor:1 | 1 (-1.38471) | -1 | -1 |
| G: -5278.76361 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.82381 HOMO: -6.53617 LUMO: -0.35375 factor:1 | 1 (-1.69451) | -1 | -1 |
| G: -5278.76361 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.65175 HOMO: -6.75659 LUMO: -0.41361 factor:1 | 1 (-1.52245) | -1 | -1 |
| G: -5278.76361 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.45471 HOMO: -6.69400 LUMO: -0.67484 factor:1 | 1 (-1.32541) | -1 | -1 |
| G: -5278.76361 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11545.10025 HOMO: -6.89264 LUMO: -0.90886 factor:1 | 1 (-1.97095) | -1 | -1 |
| G: -5278.76361 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.78348 HOMO: -6.56339 LUMO: -0.52518 factor:1 | 1 (-1.65418) | -1 | -1 |
| G: -5278.76361 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11545.11652 HOMO: -6.45726 LUMO: -0.65852 factor:1 | 1 (-1.98722) | -1 | -1 |
| G: -5278.76361 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.91499 HOMO: -6.80557 LUMO: -0.56600 factor:1 | 1 (-1.78569) | -1 | -1 |
| G: -5278.76361 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.90267 HOMO: -7.19469 LUMO: -0.91702 factor:1 | 1 (-1.77337) | -1 | -1 |
| G: -5278.76361 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.54998 HOMO: -6.41100 LUMO: 0.79185 factor:1 | 1 (-1.42068) | -1 | -1 |
| G: -5278.76361 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.35381 HOMO: -6.39195 LUMO: 0.26123 factor:1 | 1 (-1.22451) | -1 | -1 |
| G: -5278.76361 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.71654 HOMO: -6.78924 LUMO: 0.35919 factor:1 | 1 (-1.58724) | -1 | -1 |
| G: -5278.76361 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11545.30803 HOMO: -6.50624 LUMO: 0.71838 factor:1 | 1 (-2.17873) | -1 | -1 |
| G: -5278.76361 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.80443 HOMO: -6.68584 LUMO: -0.66124 factor:1 | 1 (-1.67513) | -1 | -1 |
| G: -5278.76361 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.47294 HOMO: -6.45182 LUMO: -0.48980 factor:1 | 1 (-1.34364) | -1 | -1 |
| G: -5278.76361 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.60974 HOMO: -7.18925 LUMO: -1.01498 factor:1 | 1 (-1.48044) | -1 | -1 |
| G: -5278.76361 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.94713 HOMO: -7.18925 LUMO: -0.63130 factor:1 | 1 (-1.81783) | -1 | -1 |
| G: -5278.76361 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11545.17443 HOMO: -6.66679 LUMO: -0.57960 factor:1 | 1 (-2.04513) | -1 | -1 |
| G: -5278.76361 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11545.20509 HOMO: -6.44910 LUMO: -0.30205 factor:1 | 1 (-2.07579) | -1 | -1 |
| G: -5278.76361 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.85407 HOMO: -7.23279 LUMO: 0.46804 factor:1 | 1 (-1.72477) | -1 | -1 |
| G: -5278.76361 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.56367 HOMO: -6.92802 LUMO: -0.72927 factor:1 | 1 (-0.43438) | -1 | -1 |
| G: -5278.76361 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.75766 HOMO: -6.83278 LUMO: -0.59321 factor:1 | 1 (-0.62837) | -1 | -1 |
| G: -5278.76361 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.80305 HOMO: -7.44776 LUMO: 0.27211 factor:1 | 1 (-0.67375) | -1 | -1 |
| G: -5278.76361 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.81737 HOMO: -6.80829 LUMO: -0.59865 factor:1 | 1 (-0.68807) | -1 | -1 |
| G: -5278.76361 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.38558 HOMO: -6.63686 LUMO: -0.75103 factor:1 | 1 (-0.25628) | -1 | -1 |
| G: -5278.76361 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.44871 HOMO: -6.73210 LUMO: -0.55511 factor:1 | 1 (-0.31941) | -1 | -1 |
| G: -5278.76361 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.73674 HOMO: -6.50624 LUMO: 1.58642 factor:1 | 1 (-0.60744) | -1 | -1 |
| G: -5278.76361 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.52220 HOMO: -6.79196 LUMO: 0.96328 factor:1 | 1 (-1.39290) | -1 | -1 |
| G: -5278.76361 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11545.25173 HOMO: -6.82734 LUMO: 1.23540 factor:1 | 1 (-2.12243) | -1 | -1 |
| G: -5278.76361 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.68761 HOMO: -6.90081 LUMO: 1.25444 factor:1 | 1 (-1.55831) | -1 | -1 |
| G: -5278.76361 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.85279 HOMO: -7.00965 LUMO: -1.05036 factor:1 | 1 (-1.72349) | -1 | -1 |
| G: -5278.76361 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.37433 HOMO: -7.01237 LUMO: -1.48302 factor:1 | 1 (-1.24503) | -1 | -1 |
| G: -5278.76361 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.69760 HOMO: -6.91713 LUMO: 0.93607 factor:1 | 1 (-1.56830) | -1 | -1 |
| G: -5278.76361 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.57167 HOMO: -7.02598 LUMO: 0.92247 factor:1 | 1 (-1.44237) | -1 | -1 |
| G: -5278.76361 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.75047 HOMO: -6.98516 LUMO: 1.52384 factor:1 | 1 (-1.62117) | -1 | -1 |
| G: -5278.76361 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.55953 HOMO: -6.75387 LUMO: 1.04764 factor:1 | 1 (-1.43023) | -1 | -1 |
| G: -5278.76361 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.87184 HOMO: -7.09401 LUMO: 1.19458 factor:1 | 1 (-1.74254) | -1 | -1 |
| G: -5278.76361 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.92044 HOMO: -6.88992 LUMO: -1.56193 factor:1 | 1 (-0.79114) | -1 | -1 |
| G: -5278.76361 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.82896 HOMO: -7.00149 LUMO: 0.99866 factor:1 | 1 (-0.69966) | -1 | -1 |
| G: -5278.76361 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.00466 HOMO: -7.13755 LUMO: 1.05308 factor:1 | 1 (-0.87536) | -1 | -1 |
| G: -5278.76361 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.53420 HOMO: -6.85183 LUMO: -1.42860 factor:1 | 1 (-0.40491) | -1 | -1 |
| G: -5278.76361 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.48710 HOMO: -6.63141 LUMO: -0.88981 factor:1 | 1 (-0.35780) | -1 | -1 |
| G: -5278.76361 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.78131 HOMO: -6.92258 LUMO: -0.82178 factor:1 | 1 (-0.65201) | -1 | -1 |
| G: -5278.76361 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.92733 HOMO: -6.55794 LUMO: -0.80818 factor:1 | 1 (-0.79803) | -1 | -1 |
| G: -5278.76361 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.68321 HOMO: -6.95251 LUMO: -0.97145 factor:1 | 1 (-0.55391) | -1 | -1 |
| G: -5278.76361 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.66398 HOMO: -7.37701 LUMO: 0.14150 factor:1 | 1 (-0.53468) | -1 | -1 |
| G: -5278.76361 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.73505 HOMO: -6.74842 LUMO: -0.68028 factor:1 | 1 (-0.60575) | -1 | -1 |
| G: -5278.76361 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.04126 HOMO: -6.65046 LUMO: -0.52518 factor:1 | 1 (-0.91196) | -1 | -1 |
| G: -5278.76361 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.94140 HOMO: -6.91441 LUMO: -1.13199 factor:1 | 1 (-0.81210) | -1 | -1 |
| G: -5278.76361 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.54667 HOMO: -7.00965 LUMO: -1.00682 factor:1 | 1 (-0.41737) | -1 | -1 |
| G: -5278.76361 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.42631 HOMO: -6.55794 LUMO: -0.54967 factor:1 | 1 (-0.29701) | -1 | -1 |
| G: -5278.76361 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.36068 HOMO: -6.71577 LUMO: -0.53879 factor:1 | 1 (-0.23138) | -1 | -1 |
| G: -5278.76361 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.71440 HOMO: -6.88992 LUMO: -0.55511 factor:1 | 1 (-0.58510) | -1 | -1 |
| G: -5278.76361 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.34004 HOMO: -6.74026 LUMO: -0.60681 factor:1 | 1 (-1.21074) | -1 | -1 |
| G: -5278.76361 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.47928 HOMO: -6.76747 LUMO: -0.50885 factor:1 | 1 (-1.34998) | -1 | -1 |
| G: -5278.76361 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.12886 HOMO: -6.87904 LUMO: -0.92519 factor:1 | 1 (-0.99956) | -1 | -1 |
| G: -5278.76361 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.01027 HOMO: -6.53073 LUMO: -0.53062 factor:1 | 1 (-0.88097) | -1 | -1 |
| G: -5278.76361 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.28211 HOMO: -6.97700 LUMO: -0.98505 factor:1 | 1 (-1.15281) | -1 | -1 |
| G: -5278.76361 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.17321 HOMO: -6.96884 LUMO: -0.79185 factor:1 | 1 (-1.04391) | -1 | -1 |
| G: -5278.76361 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.60359 HOMO: -6.60420 LUMO: -0.31021 factor:1 | 1 (-1.47429) | -1 | -1 |
| G: -5278.76361 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.98082 HOMO: -6.68584 LUMO: -0.63947 factor:1 | 1 (-1.85152) | -1 | -1 |
| G: -5278.76361 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.73110 HOMO: -6.41917 LUMO: -0.35103 factor:1 | 1 (-1.60180) | -1 | -1 |
| G: -5278.76361 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11545.09546 HOMO: -6.73482 LUMO: -0.70477 factor:1 | 1 (-1.96616) | -1 | -1 |
| G: -5278.76361 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11545.62096 HOMO: -6.71305 LUMO: -0.85716 factor:1 | 1 (-2.49166) | -1 | -1 |
| G: -5278.76361 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.97954 HOMO: -6.70761 LUMO: -0.63403 factor:1 | 1 (-1.85024) | -1 | -1 |
| G: -5278.76361 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.64258 HOMO: -6.37563 LUMO: -0.38640 factor:1 | 1 (-1.51328) | -1 | -1 |
| G: -5278.76361 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.71964 HOMO: -6.27495 LUMO: -0.54967 factor:1 | 1 (-1.59034) | -1 | -1 |
| G: -5278.76361 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.62353 HOMO: -6.98516 LUMO: 0.38096 factor:1 | 1 (-1.49423) | -1 | -1 |
| G: -5278.76361 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.30453 HOMO: -6.47087 LUMO: -0.40001 factor:1 | 1 (-1.17523) | -1 | -1 |
| G: -5278.76361 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.61878 HOMO: -6.59876 LUMO: 0.20681 factor:1 | 1 (-0.48948) | -1 | -1 |
| G: -5278.76361 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.58027 HOMO: -6.89809 LUMO: 0.14966 factor:1 | 1 (-0.45097) | -1 | -1 |
| G: -5278.76361 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.78920 HOMO: -6.76203 LUMO: 2.11432 factor:1 | 1 (-0.65990) | -1 | -1 |
| G: -5278.76361 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.86425 HOMO: -6.58516 LUMO: 1.75786 factor:1 | 1 (-0.73495) | -1 | -1 |
| G: -5278.76361 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.40960 HOMO: -6.37835 LUMO: 1.84493 factor:1 | 1 (-0.28030) | -1 | -1 |
| G: -5278.76361 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.51796 HOMO: -6.83550 LUMO: 1.74425 factor:1 | 1 (-0.38866) | -1 | -1 |
| G: -5278.76361 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.53989 HOMO: -6.65318 LUMO: 1.79051 factor:1 | 1 (-0.41059) | -1 | -1 |
| G: -5278.76361 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.68036 HOMO: -6.68584 LUMO: 2.11160 factor:1 | 1 (-0.55106) | -1 | -1 |
| G: -5278.76361 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.65170 HOMO: -6.36202 LUMO: 1.85037 factor:1 | 1 (-0.52240) | -1 | -1 |
| G: -5278.76361 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.71113 HOMO: -6.68312 LUMO: 2.23133 factor:1 | 1 (-0.58183) | -1 | -1 |
| G: -5278.76361 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.78414 HOMO: -6.66679 LUMO: 2.14154 factor:1 | 1 (-0.65484) | -1 | -1 |
| G: -5278.76361 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.34432 HOMO: -6.50896 LUMO: 1.92657 factor:1 | 1 (-0.21502) | -1 | -1 |
| G: -5278.76361 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.50795 HOMO: -6.63686 LUMO: 2.22317 factor:1 | 1 (-0.37865) | -1 | -1 |
| G: -5278.76361 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.49630 HOMO: -6.58788 LUMO: 2.17419 factor:1 | 1 (-0.36700) | -1 | -1 |
| G: -5278.76361 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.72180 HOMO: -6.72665 LUMO: 2.12249 factor:1 | 1 (-0.59250) | -1 | -1 |
| G: -5278.76361 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.62166 HOMO: -6.28311 LUMO: 1.91024 factor:1 | 1 (-0.49236) | -1 | -1 |
| G: -5278.76361 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.38710 HOMO: -6.56067 LUMO: 2.27487 factor:1 | 1 (-0.25780) | -1 | -1 |
| G: -5278.76361 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.24457 HOMO: -6.83006 LUMO: 2.28031 factor:1 | 1 (-0.11527) | -1 | -1 |
| G: -5278.76361 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.55472 HOMO: -6.45182 LUMO: 1.62724 factor:1 | 1 (-0.42542) | -1 | -1 |
| G: -5278.76361 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.39567 HOMO: -6.78380 LUMO: 1.83677 factor:1 | 1 (-0.26637) | -1 | -1 |
| G: -5278.76361 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.67979 HOMO: -6.23413 LUMO: 1.80956 factor:1 | 1 (-0.55049) | -1 | -1 |
| G: -5278.76361 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.86914 HOMO: -6.74298 LUMO: 2.16875 factor:1 | 1 (-1.73984) | -1 | -1 |
| G: -5278.76361 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11545.62301 HOMO: -6.81645 LUMO: 2.50073 factor:1 | 1 (-2.49371) | -1 | -1 |
| G: -5278.76361 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11545.02416 HOMO: -6.71033 LUMO: 1.96466 factor:1 | 1 (-1.89486) | -1 | -1 |
| G: -5278.76361 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.69240 HOMO: -6.83550 LUMO: 2.04358 factor:1 | 1 (-1.56310) | -1 | -1 |
| G: -5278.76361 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.68945 HOMO: -6.60965 LUMO: 2.38100 factor:1 | 1 (-0.56015) | -1 | -1 |
| G: -5278.76361 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.30051 HOMO: -6.73210 LUMO: 2.26127 factor:1 | 1 (-0.17121) | -1 | -1 |
| G: -5278.76361 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.03237 HOMO: -6.76203 LUMO: 2.13609 factor:1 | -1 (0.09693) | -1 | -1 |
| G: -5278.76361 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.45684 HOMO: -6.71033 LUMO: 2.05990 factor:1 | 1 (-0.32754) | -1 | -1 |
| G: -5278.76361 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.39175 HOMO: -6.50896 LUMO: 2.32385 factor:1 | 1 (-0.26245) | -1 | -1 |
| G: -5278.76361 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.61149 HOMO: -6.53345 LUMO: 1.74425 factor:1 | 1 (-0.48219) | -1 | -1 |
| G: -5278.76361 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11545.11636 HOMO: -6.25862 LUMO: 1.63540 factor:1 | 1 (-1.98706) | -1 | -1 |
| G: -5278.76361 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.34630 HOMO: -5.90759 LUMO: 1.78779 factor:1 | 1 (-1.21700) | -1 | -1 |
| G: -5278.76361 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.69401 HOMO: -6.09807 LUMO: 1.99732 factor:1 | 1 (-1.56471) | -1 | -1 |
| G: -5278.76361 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.31645 HOMO: -5.92392 LUMO: 1.99732 factor:1 | 1 (-1.18715) | -1 | -1 |
| G: -5278.76361 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.45458 HOMO: -6.45182 LUMO: 1.72248 factor:1 | 1 (-1.32528) | -1 | -1 |
| G: -5278.76361 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.71878 HOMO: -6.53073 LUMO: 1.82588 factor:1 | 1 (-0.58948) | -1 | -1 |
| G: -5278.76361 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.55733 HOMO: -6.40828 LUMO: 2.05174 factor:1 | 1 (-0.42804) | -1 | -1 |
| G: -5278.76361 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.65266 HOMO: -6.60420 LUMO: -0.82450 factor:1 | 1 (-0.52336) | -1 | -1 |
| G: -5278.76361 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.76243 HOMO: -6.76747 LUMO: -0.57144 factor:1 | 1 (-0.63313) | -1 | -1 |
| G: -5278.76361 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.77029 HOMO: -6.67767 LUMO: -0.59321 factor:1 | 1 (-0.64099) | -1 | -1 |
| G: -5278.76361 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.71358 HOMO: -6.65863 LUMO: -0.57416 factor:1 | 1 (-0.58428) | -1 | -1 |
| G: -5278.76361 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.53755 HOMO: -6.49808 LUMO: -0.54695 factor:1 | 1 (-0.40825) | -1 | -1 |
| G: -5278.76361 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.98352 HOMO: -6.50080 LUMO: -0.61498 factor:1 | 1 (-0.85422) | -1 | -1 |
| G: -5278.76361 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.83514 HOMO: -6.74842 LUMO: -0.51974 factor:1 | 1 (-0.70584) | -1 | -1 |
| G: -5278.76361 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.82099 HOMO: -6.13345 LUMO: 0.67756 factor:1 | 1 (-0.69169) | -1 | -1 |
| G: -5278.76361 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.78303 HOMO: -6.48719 LUMO: 0.52790 factor:1 | 1 (-0.65373) | -1 | -1 |
| G: -5278.76361 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.85236 HOMO: -6.35930 LUMO: 0.74015 factor:1 | 1 (-0.72306) | -1 | -1 |
| G: -5278.76361 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.82776 HOMO: -6.41644 LUMO: 0.22313 factor:1 | 1 (-0.69846) | -1 | -1 |
| G: -5278.76361 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.73334 HOMO: -6.85727 LUMO: -0.00272 factor:1 | 1 (-0.60404) | -1 | -1 |
| G: -5278.76361 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.82662 HOMO: -6.84638 LUMO: 0.24762 factor:1 | 1 (-0.69732) | -1 | -1 |
| G: -5278.76361 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.70569 HOMO: -6.66951 LUMO: 0.39184 factor:1 | 1 (-0.57639) | -1 | -1 |
| G: -5278.76361 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.25784 HOMO: -6.62597 LUMO: -0.65035 factor:1 | 1 (-1.12854) | -1 | -1 |
| G: -5278.76361 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.25460 HOMO: -7.13755 LUMO: 0.45715 factor:1 | 1 (-1.12530) | -1 | -1 |
| G: -5278.76361 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.04221 HOMO: -7.12666 LUMO: 0.45171 factor:1 | 1 (-0.91291) | -1 | -1 |
| G: -5278.76361 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.15890 HOMO: -6.46270 LUMO: -0.46259 factor:1 | 1 (-1.02960) | -1 | -1 |
| G: -5278.76361 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.31221 HOMO: -6.36202 LUMO: -0.29660 factor:1 | 1 (-1.18291) | -1 | -1 |
| G: -5278.76361 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.25776 HOMO: -6.28583 LUMO: 0.40545 factor:1 | 1 (-1.12846) | -1 | -1 |
| G: -5278.76361 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.75448 HOMO: -6.70761 LUMO: 0.41906 factor:1 | 1 (-0.62518) | -1 | -1 |
| G: -5278.76361 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.92202 HOMO: -6.76203 LUMO: -0.60954 factor:1 | 1 (-0.79272) | -1 | -1 |
| G: -5278.76361 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.70362 HOMO: -6.85999 LUMO: -0.75103 factor:1 | 1 (-0.57432) | -1 | -1 |
| G: -5278.76361 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.82986 HOMO: -7.19741 LUMO: -1.00954 factor:1 | 1 (-0.70056) | -1 | -1 |
| G: -5278.76361 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.94126 HOMO: -6.58243 LUMO: -0.33470 factor:1 | 1 (-0.81196) | -1 | -1 |
| G: -5278.76361 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.46454 HOMO: -7.22190 LUMO: 0.49253 factor:1 | 1 (-0.33524) | -1 | -1 |
| G: -5278.76361 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.66945 HOMO: -7.22462 LUMO: 0.51974 factor:1 | 1 (-0.54015) | -1 | -1 |
| G: -5278.76361 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.67674 HOMO: -7.08584 LUMO: -0.68301 factor:1 | 1 (-0.54744) | -1 | -1 |
| G: -5278.76361 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.74634 HOMO: -6.68584 LUMO: -0.29660 factor:1 | 1 (-0.61705) | -1 | -1 |
| G: -5278.76361 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.75372 HOMO: -6.33753 LUMO: -0.48436 factor:1 | 1 (-0.62442) | -1 | -1 |
| G: -5278.76361 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.54278 HOMO: -7.15932 LUMO: 0.55511 factor:1 | 1 (-0.41348) | -1 | -1 |
| G: -5278.76361 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.65475 HOMO: -6.57427 LUMO: 2.01908 factor:1 | 1 (-0.52545) | -1 | -1 |
| G: -5278.76361 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.75220 HOMO: -6.75659 LUMO: 2.22045 factor:1 | 1 (-0.62290) | -1 | -1 |
| G: -5278.76361 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.58223 HOMO: -6.73482 LUMO: 2.20956 factor:1 | 1 (-0.45293) | -1 | -1 |
| G: -5278.76361 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.34718 HOMO: -6.74026 LUMO: 1.76602 factor:1 | 1 (-0.21788) | -1 | -1 |
| G: -5278.76361 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.26424 HOMO: -6.95523 LUMO: 1.94834 factor:1 | 1 (-0.13494) | -1 | -1 |
| G: -5278.76361 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.50327 HOMO: -6.33209 LUMO: 1.87486 factor:1 | 1 (-0.37397) | -1 | -1 |
| G: -5278.76361 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.54321 HOMO: -6.71033 LUMO: 2.12521 factor:1 | 1 (-0.41391) | -1 | -1 |
| G: -5278.76361 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.71111 HOMO: -6.50080 LUMO: 2.04902 factor:1 | 1 (-0.58181) | -1 | -1 |
| G: -5278.76361 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.77241 HOMO: -6.76475 LUMO: 1.94017 factor:1 | 1 (-0.64311) | -1 | -1 |
| G: -5278.76361 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.89672 HOMO: -6.53073 LUMO: 2.08983 factor:1 | 1 (-0.76742) | -1 | -1 |
| G: -5278.76361 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.91005 HOMO: -6.69944 LUMO: 2.20684 factor:1 | 1 (-0.78075) | -1 | -1 |
| G: -5278.76361 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.66234 HOMO: -6.34570 LUMO: 1.80684 factor:1 | 1 (-0.53304) | -1 | -1 |
| G: -5278.76361 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.61162 HOMO: -6.78380 LUMO: 1.95922 factor:1 | 1 (-0.48232) | -1 | -1 |
| G: -5278.76361 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.72515 HOMO: -6.93618 LUMO: 1.76058 factor:1 | 1 (-0.59585) | -1 | -1 |
| G: -5278.76361 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.85339 HOMO: -6.93346 LUMO: 1.79595 factor:1 | 1 (-0.72409) | -1 | -1 |
| G: -5278.76361 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.92760 HOMO: -6.29671 LUMO: 1.75241 factor:1 | 1 (-0.79830) | -1 | -1 |
| G: -5278.76361 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.82703 HOMO: -6.77019 LUMO: 1.74697 factor:1 | 1 (-0.69773) | -1 | -1 |
| G: -5278.76361 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.77712 HOMO: -6.87360 LUMO: 1.91024 factor:1 | 1 (-0.64782) | -1 | -1 |
| G: -5278.76361 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.53306 HOMO: -6.32665 LUMO: 1.87759 factor:1 | 1 (-0.40376) | -1 | -1 |
| G: -5278.76361 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.62634 HOMO: -6.99877 LUMO: 1.99187 factor:1 | 1 (-0.49704) | -1 | -1 |
| G: -5278.76361 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.89533 HOMO: -6.72665 LUMO: 2.12521 factor:1 | 1 (-0.76603) | -1 | -1 |
| G: -5278.76361 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.70428 HOMO: -6.67767 LUMO: 2.43814 factor:1 | 1 (-0.57498) | -1 | -1 |
| G: -5278.76361 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.47521 HOMO: -6.99605 LUMO: 1.79051 factor:1 | 1 (-0.34591) | -1 | -1 |
| G: -5278.76361 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.02891 HOMO: -6.25046 LUMO: 1.77146 factor:1 | 1 (-0.89961) | -1 | -1 |
| G: -5278.76361 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.84716 HOMO: -6.30488 LUMO: 1.90480 factor:1 | 1 (-0.71786) | -1 | -1 |
| G: -5278.76361 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.59192 HOMO: -6.38379 LUMO: 1.68438 factor:1 | 1 (-0.46262) | -1 | -1 |
| G: -5278.76361 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.71326 HOMO: -6.78924 LUMO: 2.01364 factor:1 | 1 (-0.58396) | -1 | -1 |
| G: -5278.76361 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.61081 HOMO: -6.15249 LUMO: 1.98643 factor:1 | 1 (-0.48151) | -1 | -1 |
| G: -5278.76361 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.52923 HOMO: -6.19331 LUMO: 2.14154 factor:1 | 1 (-0.39993) | -1 | -1 |
| G: -5278.76361 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.77916 HOMO: -6.05998 LUMO: 2.12521 factor:1 | 1 (-0.64986) | -1 | -1 |
| G: -5278.76361 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.53412 HOMO: -6.67223 LUMO: 1.91840 factor:1 | 1 (-0.40482) | -1 | -1 |
| G: -5278.76361 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.66430 HOMO: -6.79196 LUMO: 2.18507 factor:1 | 1 (-0.53500) | -1 | -1 |
| G: -5278.76361 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.57744 HOMO: -6.93346 LUMO: 1.78235 factor:1 | 1 (-0.44814) | -1 | -1 |
| G: -5278.76361 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.70860 HOMO: -6.16882 LUMO: 1.80956 factor:1 | 1 (-0.57930) | -1 | -1 |
| G: -5278.76361 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.34734 HOMO: -6.72665 LUMO: 2.07895 factor:1 | 1 (-1.21804) | -1 | -1 |
| G: -5278.76361 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.42070 HOMO: -6.73210 LUMO: 1.97827 factor:1 | 1 (-1.29140) | -1 | -1 |
| G: -5278.76361 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.41632 HOMO: -6.84638 LUMO: 1.87214 factor:1 | 1 (-1.28702) | -1 | -1 |
| G: -5278.76361 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.37117 HOMO: -6.83006 LUMO: 2.36195 factor:1 | 1 (-1.24187) | -1 | -1 |
| G: -5278.76361 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.30306 HOMO: -6.97700 LUMO: 1.91024 factor:1 | 1 (-1.17376) | -1 | -1 |
| G: -5278.76361 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.33365 HOMO: -6.20420 LUMO: 1.81772 factor:1 | 1 (-1.20435) | -1 | -1 |
| G: -5278.76361 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.73358 HOMO: -7.09129 LUMO: 2.10344 factor:1 | 1 (-0.60428) | 1 | 1 |
| G: -5278.76361 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.71132 HOMO: -6.77564 LUMO: 2.14970 factor:1 | 1 (-0.58202) | -1 | -1 |
| G: -5278.76361 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.89078 HOMO: -6.81645 LUMO: 1.85854 factor:1 | 1 (-0.76148) | -1 | -1 |
| G: -5278.76361 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.91446 HOMO: -6.50896 LUMO: 2.04358 factor:1 | 1 (-0.78516) | -1 | -1 |
| G: -5278.76361 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.48343 HOMO: -6.89264 LUMO: 1.66262 factor:1 | 1 (-0.35413) | -1 | -1 |
| G: -5278.76361 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.55342 HOMO: -6.75931 LUMO: 2.23950 factor:1 | 1 (-0.42412) | -1 | -1 |
| G: -5278.76361 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.63459 HOMO: -6.50080 LUMO: 1.67622 factor:1 | 1 (-0.50529) | -1 | -1 |
| G: -5278.76361 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.44495 HOMO: -6.30216 LUMO: 2.24222 factor:1 | 1 (-0.31565) | -1 | -1 |
| G: -5278.76361 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.50922 HOMO: -7.18108 LUMO: 2.10072 factor:1 | 1 (-0.37993) | 1 | 1 |
| G: -5278.76361 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.61399 HOMO: -6.54162 LUMO: 2.35378 factor:1 | 1 (-0.48469) | -1 | -1 |
| G: -5278.76361 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.42971 HOMO: -5.98650 LUMO: 1.48302 factor:1 | 1 (-0.30041) | -1 | -1 |
| G: -5278.76361 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.59529 HOMO: -7.15115 LUMO: 2.14970 factor:1 | 1 (-0.46599) | 1 | 1 |
| G: -5278.76361 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.55687 HOMO: -6.45454 LUMO: 2.15786 factor:1 | 1 (-0.42757) | -1 | -1 |
| G: -5278.76361 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.74469 HOMO: -7.06952 LUMO: 2.14970 factor:1 | 1 (-0.61539) | 1 | 1 |
| G: -5278.76361 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.61045 HOMO: -6.93618 LUMO: 1.86942 factor:1 | 1 (-0.48115) | -1 | -1 |
| G: -5278.76361 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.52082 HOMO: -6.63141 LUMO: 1.92657 factor:1 | 1 (-0.39152) | -1 | -1 |
| G: -5278.76361 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.58672 HOMO: -6.51441 LUMO: -0.44355 factor:1 | 1 (-0.45742) | -1 | -1 |
| G: -5278.76361 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.32597 HOMO: -6.82734 LUMO: -1.03131 factor:1 | 1 (-1.19668) | -1 | -1 |
| G: -5278.76361 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.19033 HOMO: -6.58788 LUMO: -0.82995 factor:1 | 1 (-1.06103) | -1 | -1 |
| G: -5278.76361 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.29904 HOMO: -6.43277 LUMO: -0.40817 factor:1 | 1 (-1.16974) | -1 | -1 |
| G: -5278.76361 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.26644 HOMO: -6.78924 LUMO: -0.72110 factor:1 | 1 (-1.13714) | -1 | -1 |
| G: -5278.76361 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.27558 HOMO: -7.28177 LUMO: 0.36735 factor:1 | 1 (-1.14628) | -1 | -1 |
| G: -5278.76361 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.14072 HOMO: -6.47903 LUMO: -0.46259 factor:1 | 1 (-1.01142) | -1 | -1 |
| G: -5278.76361 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.17509 HOMO: -6.67495 LUMO: -0.75376 factor:1 | 1 (-1.04579) | -1 | -1 |
| G: -5278.76361 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.24453 HOMO: -6.71033 LUMO: -0.71838 factor:1 | 1 (-1.11523) | -1 | -1 |
| G: -5278.76361 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.10415 HOMO: -6.79740 LUMO: -0.79185 factor:1 | 1 (-0.97485) | -1 | -1 |
| G: -5278.76361 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.22766 HOMO: -6.08719 LUMO: -0.63675 factor:1 | 1 (-1.09836) | -1 | -1 |
| G: -5278.76361 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.22309 HOMO: -6.84094 LUMO: 0.42994 factor:1 | 1 (-1.09379) | -1 | -1 |
| G: -5278.76361 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.27395 HOMO: -6.59604 LUMO: 0.25851 factor:1 | 1 (-1.14465) | -1 | -1 |
| G: -5278.76361 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.52830 HOMO: -6.82462 LUMO: 0.08708 factor:1 | 1 (-0.39900) | -1 | -1 |
| G: -5278.76361 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.73160 HOMO: -6.54706 LUMO: 0.44082 factor:1 | 1 (-0.60230) | -1 | -1 |
| G: -5278.76361 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.55997 HOMO: -6.99333 LUMO: 0.32109 factor:1 | 1 (-0.43067) | -1 | -1 |
| G: -5278.76361 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.77889 HOMO: -6.29944 LUMO: -0.57144 factor:1 | 1 (-0.64959) | -1 | -1 |
| G: -5278.76361 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.53752 HOMO: -6.57699 LUMO: -0.46531 factor:1 | 1 (-0.40823) | -1 | -1 |
| G: -5278.76361 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.26405 HOMO: -6.24773 LUMO: -0.53879 factor:1 | 1 (-0.13475) | -1 | -1 |
| G: -5278.76361 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.39494 HOMO: -6.96067 LUMO: -0.67212 factor:1 | 1 (-0.26564) | -1 | -1 |
| G: -5278.76361 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.51404 HOMO: -7.24095 LUMO: -0.09252 factor:1 | 1 (-0.38474) | -1 | -1 |
| G: -5278.76361 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.28917 HOMO: -6.33481 LUMO: -0.46531 factor:1 | 1 (-0.15987) | -1 | -1 |
| G: -5278.76361 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.70814 HOMO: -6.43549 LUMO: -0.33198 factor:1 | 1 (-0.57884) | -1 | -1 |
| G: -5278.76361 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.89261 HOMO: -6.53073 LUMO: 0.44899 factor:1 | 1 (-0.76331) | -1 | -1 |
| G: -5278.76361 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.95484 HOMO: -6.69128 LUMO: 0.47620 factor:1 | 1 (-0.82554) | -1 | -1 |
| G: -5278.76361 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.10099 HOMO: -6.65318 LUMO: 0.52246 factor:1 | 1 (-0.97169) | -1 | -1 |
| G: -5278.76361 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.02284 HOMO: -6.71305 LUMO: 0.41089 factor:1 | 1 (-0.89354) | -1 | -1 |
| G: -5278.76361 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.94523 HOMO: -6.70216 LUMO: 0.19864 factor:1 | 1 (-0.81593) | -1 | -1 |
| G: -5278.76361 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.88042 HOMO: -6.41100 LUMO: 0.34558 factor:1 | 1 (-0.75112) | -1 | -1 |
| G: -5278.76361 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.01908 HOMO: -7.01237 LUMO: 0.02993 factor:1 | 1 (-0.88979) | -1 | -1 |
| G: -5278.76361 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.00055 HOMO: -6.85999 LUMO: 0.18776 factor:1 | 1 (-0.87125) | -1 | -1 |
| G: -5278.76361 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.73825 HOMO: -6.62869 LUMO: 0.48708 factor:1 | 1 (-1.60895) | -1 | -1 |
| G: -5278.76361 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.53022 HOMO: -6.43821 LUMO: -0.45715 factor:1 | 1 (-1.40092) | -1 | -1 |
| G: -5278.76361 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.43972 HOMO: -6.43277 LUMO: -0.72110 factor:1 | 1 (-1.31042) | -1 | -1 |
| G: -5278.76361 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.42777 HOMO: -7.10761 LUMO: 0.43266 factor:1 | 1 (-1.29847) | -1 | -1 |
| G: -5278.76361 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.57401 HOMO: -6.57699 LUMO: -0.61498 factor:1 | 1 (-1.44471) | -1 | -1 |
| G: -5278.76361 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.52013 HOMO: -6.82189 LUMO: -0.75648 factor:1 | 1 (-1.39083) | -1 | -1 |
| G: -5278.76361 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.61678 HOMO: -6.55794 LUMO: -0.67212 factor:1 | 1 (-1.48748) | -1 | -1 |
| G: -5278.76361 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.33876 HOMO: -6.69128 LUMO: 1.88575 factor:1 | 1 (-1.20946) | -1 | -1 |
| G: -5278.76361 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.50293 HOMO: -6.65591 LUMO: 1.70888 factor:1 | 1 (-1.37363) | -1 | -1 |
| G: -5278.76361 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.40753 HOMO: -6.58788 LUMO: 1.68438 factor:1 | 1 (-1.27823) | -1 | -1 |
| G: -5278.76361 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.23278 HOMO: -6.46270 LUMO: 1.72520 factor:1 | 1 (-1.10348) | -1 | -1 |
| G: -5278.76361 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.44761 HOMO: -6.57427 LUMO: 1.73881 factor:1 | 1 (-1.31831) | -1 | -1 |
| G: -5278.76361 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.53373 HOMO: -6.45182 LUMO: 1.75241 factor:1 | 1 (-1.40443) | -1 | -1 |
| G: -5278.76361 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.34404 HOMO: -6.51441 LUMO: 1.78779 factor:1 | 1 (-1.21474) | -1 | -1 |
| G: -5278.76361 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.32255 HOMO: -6.67495 LUMO: 2.11705 factor:1 | 1 (-1.19325) | -1 | -1 |
| G: -5278.76361 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.28578 HOMO: -6.22597 LUMO: 1.96466 factor:1 | 1 (-1.15648) | -1 | -1 |
| G: -5278.76361 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.38878 HOMO: -6.68040 LUMO: 2.30753 factor:1 | 1 (-1.25948) | -1 | -1 |
| G: -5278.76361 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.31759 HOMO: -6.65046 LUMO: 2.18235 factor:1 | 1 (-1.18829) | -1 | -1 |
| G: -5278.76361 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.81328 HOMO: -6.38651 LUMO: 1.76874 factor:1 | 1 (-0.68399) | -1 | -1 |
| G: -5278.76361 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.64868 HOMO: -6.41644 LUMO: 2.09256 factor:1 | 1 (-0.51938) | -1 | -1 |
| G: -5278.76361 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.80425 HOMO: -6.14977 LUMO: 2.28031 factor:1 | 1 (-0.67495) | -1 | -1 |
| G: -5278.76361 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.81862 HOMO: -6.70489 LUMO: 2.43814 factor:1 | 1 (-0.68932) | -1 | -1 |
| G: -5278.76361 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.92727 HOMO: -6.78924 LUMO: 2.27215 factor:1 | 1 (-0.79797) | -1 | -1 |
| G: -5278.76361 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.94036 HOMO: -6.86271 LUMO: 2.31025 factor:1 | 1 (-0.81106) | -1 | -1 |
| G: -5278.76361 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.69644 HOMO: -6.51168 LUMO: 2.04630 factor:1 | 1 (-0.56714) | -1 | -1 |
| G: -5278.76361 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.61625 HOMO: -6.72665 LUMO: 2.13337 factor:1 | 1 (-0.48695) | -1 | -1 |
| G: -5278.76361 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.56675 HOMO: -6.45998 LUMO: 2.16058 factor:1 | 1 (-0.43745) | -1 | -1 |
| G: -5278.76361 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.82237 HOMO: -6.83822 LUMO: 2.20684 factor:1 | 1 (-0.69307) | -1 | -1 |
| G: -5278.76361 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11545.09940 HOMO: -6.68856 LUMO: 2.19324 factor:1 | 1 (-1.97010) | -1 | -1 |
| G: -5278.76361 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11545.04095 HOMO: -6.71577 LUMO: 2.16058 factor:1 | 1 (-1.91165) | -1 | -1 |
| G: -5278.76361 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11545.08430 HOMO: -6.82462 LUMO: 1.90208 factor:1 | 1 (-1.95500) | -1 | -1 |
| G: -5278.76361 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11545.18349 HOMO: -6.61509 LUMO: 2.23950 factor:1 | 1 (-2.05419) | -1 | -1 |
| G: -5278.76361 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.90615 HOMO: -6.73754 LUMO: 1.84221 factor:1 | 1 (-1.77685) | -1 | -1 |
| G: -5278.76361 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.69861 HOMO: -6.56611 LUMO: 1.94561 factor:1 | 1 (-1.56931) | -1 | -1 |
| G: -5278.76361 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.83801 HOMO: -6.67767 LUMO: 1.51840 factor:1 | 1 (-1.70871) | -1 | -1 |
| G: -5278.76361 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.61850 HOMO: -6.35658 LUMO: 2.16603 factor:1 | 1 (-1.48920) | -1 | -1 |
| G: -5278.76361 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11545.02950 HOMO: -6.35114 LUMO: 2.08983 factor:1 | 1 (-1.90020) | -1 | -1 |
| G: -5278.76361 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.78979 HOMO: -6.35114 LUMO: 2.10616 factor:1 | 1 (-1.66049) | -1 | -1 |
| G: -5278.76361 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.92590 HOMO: -6.71305 LUMO: 2.01636 factor:1 | 1 (-1.79660) | -1 | -1 |
| G: -5278.76361 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.85921 HOMO: -6.24773 LUMO: 1.98915 factor:1 | 1 (-1.72991) | -1 | -1 |
| G: -5278.76361 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.96207 HOMO: -6.53617 LUMO: 2.42726 factor:1 | 1 (-1.83277) | -1 | -1 |
| G: -5278.76361 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.53882 HOMO: -6.59332 LUMO: 1.82316 factor:1 | 1 (-1.40952) | -1 | -1 |
| G: -5278.76361 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.69210 HOMO: -6.41372 LUMO: 1.77418 factor:1 | 1 (-1.56280) | -1 | -1 |
| G: -5278.76361 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.62544 HOMO: -6.40284 LUMO: 1.88575 factor:1 | 1 (-1.49614) | -1 | -1 |
| G: -5278.76361 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.19057 HOMO: -6.11168 LUMO: 1.70888 factor:1 | 1 (-1.06127) | -1 | -1 |
| G: -5278.76361 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.51177 HOMO: -6.44910 LUMO: 2.23405 factor:1 | 1 (-1.38247) | -1 | -1 |
| G: -5278.76361 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.35645 HOMO: -6.24773 LUMO: 2.12793 factor:1 | 1 (-1.22715) | -1 | -1 |
| G: -5278.76361 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.53256 HOMO: -6.07358 LUMO: 1.89663 factor:1 | 1 (-1.40326) | -1 | -1 |
| G: -5278.76361 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.62435 HOMO: -6.66679 LUMO: 1.96738 factor:1 | 1 (-1.49505) | -1 | -1 |
| G: -5278.76361 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.53689 HOMO: -6.68312 LUMO: 1.78235 factor:1 | 1 (-1.40759) | -1 | -1 |
| G: -5278.76361 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.28328 HOMO: -6.70761 LUMO: 1.97555 factor:1 | 1 (-1.15398) | -1 | -1 |
| G: -5278.76361 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.12352 HOMO: -6.15794 LUMO: 2.00548 factor:1 | 1 (-0.99422) | -1 | -1 |
| G: -5278.76361 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.29830 HOMO: -6.52257 LUMO: 1.96738 factor:1 | 1 (-1.16900) | -1 | -1 |
| G: -5278.76361 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.40540 HOMO: -6.25590 LUMO: 1.86670 factor:1 | 1 (-1.27611) | -1 | -1 |
| G: -5278.76361 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.31463 HOMO: -6.30216 LUMO: 1.84765 factor:1 | 1 (-1.18533) | -1 | -1 |
| G: -5278.76361 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.36380 HOMO: -6.76747 LUMO: 2.20956 factor:1 | 1 (-1.23450) | -1 | -1 |
| G: -5278.76361 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.60440 HOMO: -6.14161 LUMO: 1.80684 factor:1 | 1 (-1.47510) | -1 | -1 |
| G: -5278.76361 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11545.01442 HOMO: -6.81373 LUMO: 1.91024 factor:1 | 1 (-1.88512) | -1 | -1 |
| G: -5278.76361 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.90544 HOMO: -6.81917 LUMO: 2.34834 factor:1 | 1 (-1.77614) | -1 | -1 |
| G: -5278.76361 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.65382 HOMO: -6.72121 LUMO: 1.90208 factor:1 | 1 (-1.52452) | -1 | -1 |
| G: -5278.76361 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.80884 HOMO: -7.51851 LUMO: 0.26939 factor:1 | 1 (-1.67954) | -1 | -1 |
| G: -5278.76361 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11545.00185 HOMO: -6.65318 LUMO: -0.57144 factor:1 | 1 (-1.87255) | -1 | -1 |
| G: -5278.76361 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.94830 HOMO: -6.77564 LUMO: -0.72654 factor:1 | 1 (-1.81900) | -1 | -1 |
| G: -5278.76361 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.77523 HOMO: -6.80557 LUMO: -0.60954 factor:1 | 1 (-1.64594) | -1 | -1 |
| G: -5278.76361 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.94052 HOMO: -7.35524 LUMO: 0.27483 factor:1 | 1 (-1.81122) | -1 | -1 |
| G: -5278.76361 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.88182 HOMO: -6.94979 LUMO: -0.83811 factor:1 | 1 (-1.75252) | -1 | -1 |
| G: -5278.76361 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.72514 HOMO: -6.13345 LUMO: -0.67212 factor:1 | 1 (-1.59584) | -1 | -1 |
| G: -5278.76361 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.48141 HOMO: -6.47359 LUMO: -0.59321 factor:1 | 1 (-1.35211) | -1 | -1 |
| G: -5278.76361 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.50070 HOMO: -6.52257 LUMO: -0.54695 factor:1 | 1 (-1.37140) | -1 | -1 |
| G: -5278.76361 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.20418 HOMO: -6.61781 LUMO: -0.69661 factor:1 | 1 (-1.07488) | -1 | -1 |
| G: -5278.76361 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.57871 HOMO: -6.77564 LUMO: -0.80001 factor:1 | 1 (-1.44941) | -1 | -1 |
| G: -5278.76361 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.72843 HOMO: -7.35252 LUMO: -1.00410 factor:1 | 1 (-1.59913) | -1 | -1 |
| G: -5278.76361 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.95818 HOMO: -6.35386 LUMO: -0.38912 factor:1 | 1 (-1.82888) | -1 | -1 |
| G: -5278.76361 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11545.61299 HOMO: -6.80285 LUMO: -0.52246 factor:1 | 1 (-2.48369) | -1 | -1 |
| G: -5278.76361 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11545.72135 HOMO: -7.23279 LUMO: 0.30477 factor:1 | 1 (-2.59205) | -1 | -1 |
| G: -5278.76361 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11546.30694 HOMO: -7.13483 LUMO: -0.76192 factor:1 | 1 (-3.17764) | -1 | -1 |
| G: -5278.76361 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11545.61261 HOMO: -6.71849 LUMO: -0.48164 factor:1 | 1 (-2.48331) | -1 | -1 |
| G: -5278.76361 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11545.48581 HOMO: -6.85455 LUMO: -0.69389 factor:1 | 1 (-2.35651) | -1 | -1 |
| G: -5278.76361 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11545.63073 HOMO: -6.96339 LUMO: -0.73743 factor:1 | 1 (-2.50143) | -1 | -1 |
| G: -5278.76361 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11546.20781 HOMO: -7.50490 LUMO: 0.28844 factor:1 | 1 (-3.07851) | -1 | -1 |
| G: -5278.76361 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11545.55566 HOMO: -6.63958 LUMO: -0.50069 factor:1 | 1 (-2.42636) | -1 | -1 |
| G: -5278.76361 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11545.72644 HOMO: -6.78924 LUMO: -0.69661 factor:1 | 1 (-2.59714) | -1 | -1 |
| G: -5278.76361 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11545.13791 HOMO: -7.44776 LUMO: 0.33742 factor:1 | 1 (-2.00861) | -1 | -1 |
| G: -5278.76361 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11545.16346 HOMO: -6.15249 LUMO: 0.66396 factor:1 | 1 (-2.03416) | -1 | -1 |
| G: -5278.76361 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11545.03159 HOMO: -6.17426 LUMO: 0.55511 factor:1 | 1 (-1.90229) | -1 | -1 |
| G: -5278.76361 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.97788 HOMO: -6.83550 LUMO: 0.28844 factor:1 | 1 (-1.84858) | -1 | -1 |
| G: -5278.76361 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11545.80325 HOMO: -6.32393 LUMO: 0.47620 factor:1 | 1 (-2.67395) | -1 | -1 |
| G: -5278.76361 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11545.77392 HOMO: -6.32937 LUMO: 0.45987 factor:1 | 1 (-2.64462) | -1 | -1 |
| G: -5278.76361 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11545.65174 HOMO: -7.37429 LUMO: 0.09252 factor:1 | 1 (-2.52244) | -1 | -1 |
| G: -5278.76361 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11545.69403 HOMO: -6.54434 LUMO: -0.39729 factor:1 | 1 (-2.56473) | -1 | -1 |
| G: -5278.76361 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11545.46708 HOMO: -7.35524 LUMO: 0.28028 factor:1 | 1 (-2.33778) | -1 | -1 |
| G: -5278.76361 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.86748 HOMO: -6.95523 LUMO: -0.86804 factor:1 | 1 (-1.73818) | -1 | -1 |
| G: -5278.76361 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.80370 HOMO: -6.63958 LUMO: -0.65307 factor:1 | 1 (-1.67440) | -1 | -1 |
| G: -5278.76361 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.93143 HOMO: -6.73482 LUMO: -0.67212 factor:1 | 1 (-1.80213) | -1 | -1 |
| G: -5278.76361 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.72530 HOMO: -6.37835 LUMO: -0.53606 factor:1 | 1 (-1.59600) | -1 | -1 |
| G: -5278.76361 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.56016 HOMO: -6.71849 LUMO: -0.61226 factor:1 | 1 (-1.43086) | -1 | -1 |
| G: -5278.76361 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.85107 HOMO: -6.68584 LUMO: -1.11022 factor:1 | 1 (-1.72177) | -1 | -1 |
| G: -5278.76361 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.93820 HOMO: -6.80285 LUMO: -0.79185 factor:1 | 1 (-1.80890) | -1 | -1 |
| G: -5278.76361 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11545.34431 HOMO: -7.14571 LUMO: -0.94696 factor:1 | 1 (-2.21501) | -1 | -1 |
| G: -5278.76361 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11545.38673 HOMO: -7.16204 LUMO: -0.66124 factor:1 | 1 (-2.25743) | -1 | -1 |
| G: -5278.76361 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11545.23916 HOMO: -6.54978 LUMO: -0.54967 factor:1 | 1 (-2.10986) | -1 | -1 |
| G: -5278.76361 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11545.18738 HOMO: -6.75114 LUMO: -0.70750 factor:1 | 1 (-2.05808) | -1 | -1 |
| G: -5278.76361 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11545.34417 HOMO: -7.22190 LUMO: 0.39184 factor:1 | 1 (-2.21487) | -1 | -1 |
| G: -5278.76361 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.93238 HOMO: -7.43959 LUMO: 0.30477 factor:1 | 1 (-1.80308) | -1 | -1 |
| G: -5278.76361 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.91935 HOMO: -6.87360 LUMO: -0.77552 factor:1 | 1 (-1.79005) | -1 | -1 |
| G: -5278.76361 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.83437 HOMO: -6.82734 LUMO: -0.59593 factor:1 | 1 (-1.70507) | -1 | -1 |
| G: -5278.76361 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.65205 HOMO: -6.65318 LUMO: -0.46259 factor:1 | 1 (-1.52275) | -1 | -1 |
| G: -5278.76361 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.81866 HOMO: -7.05863 LUMO: -1.17009 factor:1 | 1 (-1.68936) | -1 | -1 |
| G: -5278.76361 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.64198 HOMO: -6.57427 LUMO: -0.48708 factor:1 | 1 (-1.51268) | -1 | -1 |
| G: -5278.76361 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.82909 HOMO: -6.60420 LUMO: -0.38096 factor:1 | 1 (-1.69979) | -1 | -1 |
| G: -5278.76361 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.64587 HOMO: -6.72121 LUMO: -0.66668 factor:1 | 1 (-1.51657) | -1 | -1 |
| G: -5278.76361 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.69102 HOMO: -6.52257 LUMO: -0.19320 factor:1 | 1 (-1.56172) | -1 | -1 |
| G: -5278.76361 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.57904 HOMO: -6.28039 LUMO: -0.27211 factor:1 | 1 (-1.44974) | -1 | -1 |
| G: -5278.76361 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.71157 HOMO: -6.71849 LUMO: -0.42722 factor:1 | 1 (-0.58227) | -1 | -1 |
| G: -5278.76361 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.66493 HOMO: -6.27495 LUMO: 0.27756 factor:1 | 1 (-0.53563) | -1 | -1 |
| G: -5278.76361 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.91549 HOMO: -6.21780 LUMO: 0.46531 factor:1 | 1 (-0.78619) | -1 | -1 |
| G: -5278.76361 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.66779 HOMO: -6.52257 LUMO: -0.64491 factor:1 | 1 (-0.53849) | -1 | -1 |
| G: -5278.76361 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.70079 HOMO: -6.73754 LUMO: 1.83133 factor:1 | 1 (-0.57149) | -1 | -1 |
| G: -5278.76361 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.94336 HOMO: -6.67223 LUMO: 1.88847 factor:1 | 1 (-0.81406) | -1 | -1 |
| G: -5278.76361 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.52046 HOMO: -6.82189 LUMO: 1.59187 factor:1 | 1 (-0.39116) | -1 | -1 |
| G: -5278.76361 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.68515 HOMO: -6.43277 LUMO: 1.76330 factor:1 | 1 (-0.55585) | -1 | -1 |
| G: -5278.76361 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.49067 HOMO: -6.48175 LUMO: 1.77962 factor:1 | 1 (-0.36137) | -1 | -1 |
| G: -5278.76361 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.66022 HOMO: -6.50352 LUMO: 1.68438 factor:1 | 1 (-0.53092) | -1 | -1 |
| G: -5278.76361 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.70844 HOMO: -6.31576 LUMO: 2.03813 factor:1 | 1 (-0.57914) | -1 | -1 |
| G: -5278.76361 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.86194 HOMO: -6.27495 LUMO: 1.99459 factor:1 | 1 (-0.73264) | -1 | -1 |
| G: -5278.76361 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.63780 HOMO: -6.23957 LUMO: 2.17147 factor:1 | 1 (-0.50850) | -1 | -1 |
| G: -5278.76361 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.73334 HOMO: -6.78108 LUMO: 2.16875 factor:1 | 1 (-0.60404) | -1 | -1 |
| G: -5278.76361 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.47042 HOMO: -6.34297 LUMO: 2.10344 factor:1 | 1 (-0.34112) | -1 | -1 |
| G: -5278.76361 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.66640 HOMO: -6.30216 LUMO: 2.00004 factor:1 | 1 (-0.53710) | -1 | -1 |
| G: -5278.76361 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.79383 HOMO: -6.72665 LUMO: 2.09528 factor:1 | 1 (-0.66453) | -1 | -1 |
| G: -5278.76361 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.53709 HOMO: -6.86543 LUMO: 1.91568 factor:1 | 1 (-0.40779) | -1 | -1 |
| G: -5278.76361 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.79005 HOMO: -5.83956 LUMO: 1.89391 factor:1 | 1 (-0.66075) | -1 | -1 |
| G: -5278.76361 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.72360 HOMO: -6.42189 LUMO: 2.03269 factor:1 | 1 (-0.59430) | -1 | -1 |
| G: -5278.76361 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.89641 HOMO: -6.07630 LUMO: 1.80956 factor:1 | 1 (-1.76711) | -1 | -1 |
| G: -5278.76361 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.80533 HOMO: -6.43277 LUMO: 1.81772 factor:1 | 1 (-1.67603) | -1 | -1 |
| G: -5278.76361 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.96762 HOMO: -7.03959 LUMO: 1.78779 factor:1 | 1 (-1.83832) | -1 | -1 |
| G: -5278.76361 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.83080 HOMO: -6.72121 LUMO: 2.29664 factor:1 | 1 (-1.70150) | -1 | -1 |
| G: -5278.76361 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.59840 HOMO: -6.62869 LUMO: 2.04630 factor:1 | 1 (-0.46910) | -1 | -1 |
| G: -5278.76361 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.61497 HOMO: -6.63958 LUMO: 1.84221 factor:1 | 1 (-0.48567) | -1 | -1 |
| G: -5278.76361 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.42609 HOMO: -6.70761 LUMO: 1.67350 factor:1 | 1 (-0.29679) | -1 | -1 |
| G: -5278.76361 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.42433 HOMO: -6.00283 LUMO: 1.64357 factor:1 | 1 (-0.29503) | -1 | -1 |
| G: -5278.76361 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.53586 HOMO: -6.48719 LUMO: 1.70343 factor:1 | 1 (-0.40657) | -1 | -1 |
| G: -5278.76361 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.56150 HOMO: -6.13345 LUMO: 1.44492 factor:1 | 1 (-0.43220) | -1 | -1 |
| G: -5278.76361 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.60895 HOMO: -6.11168 LUMO: 1.70071 factor:1 | 1 (-0.47966) | -1 | -1 |
| G: -5278.76361 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11545.28303 HOMO: -6.09535 LUMO: 1.82316 factor:1 | 1 (-2.15373) | -1 | -1 |
| G: -5278.76361 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.60873 HOMO: -6.81101 LUMO: 1.63540 factor:1 | 1 (-1.47943) | -1 | -1 |
| G: -5278.76361 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.59085 HOMO: -6.80013 LUMO: 2.12249 factor:1 | 1 (-1.46155) | -1 | -1 |
| G: -5278.76361 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.45882 HOMO: -6.48447 LUMO: 1.94561 factor:1 | 1 (-1.32952) | -1 | -1 |
| G: -5278.76361 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.49980 HOMO: -6.72393 LUMO: 2.06534 factor:1 | 1 (-1.37050) | -1 | -1 |
| G: -5278.76361 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.38192 HOMO: -6.34570 LUMO: 1.98915 factor:1 | 1 (-1.25262) | -1 | -1 |
| G: -5278.76361 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.57422 HOMO: -6.31304 LUMO: 1.87759 factor:1 | 1 (-1.44492) | -1 | -1 |
| G: -5278.76361 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.73820 HOMO: -6.77564 LUMO: 1.81228 factor:1 | 1 (-1.60890) | -1 | -1 |
| G: -5278.76361 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.69828 HOMO: -6.58516 LUMO: 2.34834 factor:1 | 1 (-1.56898) | -1 | -1 |
| G: -5278.76361 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.54682 HOMO: -6.68040 LUMO: 2.20412 factor:1 | 1 (-1.41752) | -1 | -1 |
| G: -5278.76361 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.50519 HOMO: -6.20964 LUMO: 2.17147 factor:1 | 1 (-1.37589) | -1 | -1 |
| G: -5278.76361 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.33776 HOMO: -6.54706 LUMO: 2.03813 factor:1 | 1 (-1.20846) | -1 | -1 |
| G: -5278.76361 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.18099 HOMO: -6.54162 LUMO: 2.17419 factor:1 | 1 (-1.05169) | -1 | -1 |
| G: -5278.76361 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.52456 HOMO: -6.75659 LUMO: 2.22589 factor:1 | 1 (-1.39526) | -1 | -1 |
| G: -5278.76361 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.49849 HOMO: -6.59604 LUMO: 2.59325 factor:1 | 1 (-1.36920) | -1 | -1 |
| G: -5278.76361 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.43613 HOMO: -6.11712 LUMO: 2.02181 factor:1 | 1 (-1.30683) | -1 | -1 |
| G: -5278.76361 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.56584 HOMO: -6.63141 LUMO: 2.09256 factor:1 | 1 (-1.43654) | -1 | -1 |
| G: -5278.76361 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.43183 HOMO: -6.61781 LUMO: 1.86126 factor:1 | 1 (-1.30253) | -1 | -1 |
| G: -5278.76361 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.52630 HOMO: -6.63958 LUMO: 1.77146 factor:1 | 1 (-1.39701) | -1 | -1 |
| G: -5278.76361 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.28083 HOMO: -6.60420 LUMO: 1.54561 factor:1 | 1 (-1.15153) | -1 | -1 |
| G: -5278.76361 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.12899 HOMO: -6.52529 LUMO: 2.05174 factor:1 | 1 (-0.99969) | -1 | -1 |
| G: -5278.76361 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.37572 HOMO: -6.80285 LUMO: 2.13609 factor:1 | 1 (-1.24642) | -1 | -1 |
| G: -5278.76361 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.48024 HOMO: -6.51168 LUMO: 2.25855 factor:1 | 1 (-1.35094) | -1 | -1 |
| G: -5278.76361 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.45833 HOMO: -6.64774 LUMO: 2.46263 factor:1 | 1 (-1.32903) | -1 | -1 |
| G: -5278.76361 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.30935 HOMO: -6.40828 LUMO: 1.99732 factor:1 | 1 (-1.18005) | -1 | -1 |
| G: -5278.76361 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.39950 HOMO: -5.97562 LUMO: 1.56465 factor:1 | 1 (-1.27020) | -1 | -1 |
| G: -5278.76361 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.09675 HOMO: -6.75659 LUMO: 2.23405 factor:1 | 1 (-0.96745) | -1 | -1 |
| G: -5278.76361 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.21667 HOMO: -6.68584 LUMO: 2.09528 factor:1 | 1 (-1.08737) | -1 | -1 |
| G: -5278.76361 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.49765 HOMO: -6.86543 LUMO: 1.95106 factor:1 | 1 (-1.36835) | -1 | -1 |
| G: -5278.76361 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.28208 HOMO: -6.47359 LUMO: 1.82316 factor:1 | 1 (-1.15278) | -1 | -1 |
| G: -5278.76361 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.94619 HOMO: -6.87632 LUMO: 2.08439 factor:1 | 1 (-0.81689) | -1 | -1 |
| G: -5278.76361 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.38584 HOMO: -6.33753 LUMO: 2.16603 factor:1 | 1 (-1.25654) | -1 | -1 |
| G: -5278.76361 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.37017 HOMO: -6.92258 LUMO: 1.72248 factor:1 | 1 (-1.24087) | -1 | -1 |
| G: -5278.76361 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.56255 HOMO: -6.62597 LUMO: 2.10344 factor:1 | 1 (-1.43325) | -1 | -1 |
| G: -5278.76361 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.25128 HOMO: -6.63141 LUMO: 1.94017 factor:1 | 1 (-1.12198) | -1 | -1 |
| G: -5278.76361 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.72179 HOMO: -6.48447 LUMO: 1.91840 factor:1 | 1 (-1.59249) | -1 | -1 |
| G: -5278.76361 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.30189 HOMO: -6.41372 LUMO: 1.61364 factor:1 | 1 (-1.17259) | -1 | -1 |
| G: -5278.76361 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.55814 HOMO: -6.37291 LUMO: 1.79051 factor:1 | 1 (-1.42884) | -1 | -1 |
| G: -5278.76361 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.69262 HOMO: -6.13073 LUMO: 1.77962 factor:1 | 1 (-1.56332) | -1 | -1 |
| G: -5278.76361 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.37131 HOMO: -6.13073 LUMO: 1.98915 factor:1 | 1 (-1.24201) | -1 | -1 |
| G: -5278.76361 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.52018 HOMO: -6.44094 LUMO: 1.58370 factor:1 | 1 (-1.39088) | -1 | -1 |
| G: -5278.76361 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.08624 HOMO: -6.87087 LUMO: -0.82995 factor:1 | 1 (-0.95694) | -1 | -1 |
| G: -5278.76361 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.53512 HOMO: -6.67223 LUMO: 1.08029 factor:1 | 1 (-1.40582) | -1 | -1 |
| G: -5278.76361 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.49101 HOMO: -6.82462 LUMO: 0.91702 factor:1 | 1 (-1.36171) | -1 | -1 |
| G: -5278.76361 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.30668 HOMO: -6.65863 LUMO: 1.52656 factor:1 | 1 (-1.17738) | -1 | -1 |
| G: -5278.76361 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.10736 HOMO: -6.78924 LUMO: 0.86260 factor:1 | 1 (-0.97806) | -1 | -1 |
| G: -5278.76361 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.91383 HOMO: -6.68584 LUMO: 0.94424 factor:1 | 1 (-0.78453) | -1 | -1 |
| G: -5278.76361 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.32233 HOMO: -6.58788 LUMO: 1.00138 factor:1 | 1 (-1.19303) | -1 | -1 |
| G: -5278.76361 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.33830 HOMO: -6.79740 LUMO: 0.91430 factor:1 | 1 (-1.20900) | -1 | -1 |
| G: -5278.76361 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.06679 HOMO: -6.67223 LUMO: 0.80274 factor:1 | 1 (-0.93749) | -1 | -1 |
| G: -5278.76361 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.24605 HOMO: -6.95251 LUMO: 0.90614 factor:1 | 1 (-1.11676) | -1 | -1 |
| G: -5278.76361 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.52867 HOMO: -7.19469 LUMO: 1.34152 factor:1 | 1 (-1.39937) | -1 | -1 |
| G: -5278.76361 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.09917 HOMO: -6.59332 LUMO: -0.76464 factor:1 | 1 (-0.96987) | -1 | -1 |
| G: -5278.76361 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.53025 HOMO: -6.77564 LUMO: -0.90886 factor:1 | 1 (-1.40095) | -1 | -1 |
| G: -5278.76361 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.39509 HOMO: -6.57971 LUMO: -0.41633 factor:1 | 1 (-1.26579) | -1 | -1 |
| G: -5278.76361 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.22584 HOMO: -6.68856 LUMO: -0.58232 factor:1 | 1 (-1.09654) | -1 | -1 |
| G: -5278.76361 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.42892 HOMO: -6.87087 LUMO: -0.71022 factor:1 | 1 (-1.29962) | -1 | -1 |
| G: -5278.76361 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.93522 HOMO: -6.67767 LUMO: -0.74559 factor:1 | 1 (-0.80592) | -1 | -1 |
| G: -5278.76361 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.43727 HOMO: -6.68040 LUMO: -0.65307 factor:1 | 1 (-1.30797) | -1 | -1 |
| G: -5278.76361 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.39256 HOMO: -6.32937 LUMO: 0.80274 factor:1 | 1 (-1.26326) | -1 | -1 |
| G: -5278.76361 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.59082 HOMO: -6.29671 LUMO: 0.82723 factor:1 | 1 (-1.46152) | -1 | -1 |
| G: -5278.76361 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.11862 HOMO: -6.67767 LUMO: 0.59321 factor:1 | 1 (-0.98932) | -1 | -1 |
| G: -5278.76361 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.45898 HOMO: -6.77836 LUMO: 0.50341 factor:1 | 1 (-1.32968) | -1 | -1 |
| G: -5278.76361 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.34747 HOMO: -6.61781 LUMO: 0.42450 factor:1 | 1 (-1.21817) | -1 | -1 |
| G: -5278.76361 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.47637 HOMO: -6.83278 LUMO: 0.39457 factor:1 | 1 (-1.34707) | -1 | -1 |
| G: -5278.76361 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.20018 HOMO: -6.56883 LUMO: 0.64219 factor:1 | 1 (-1.07088) | -1 | -1 |
| G: -5278.76361 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.29378 HOMO: -6.71577 LUMO: 0.40001 factor:1 | 1 (-1.16448) | -1 | -1 |
| G: -5278.76361 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.16973 HOMO: -6.86543 LUMO: -0.74287 factor:1 | 1 (-1.04043) | -1 | -1 |
| G: -5278.76361 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.43441 HOMO: -6.68584 LUMO: -0.69389 factor:1 | 1 (-1.30511) | -1 | -1 |
| G: -5278.76361 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.47977 HOMO: -6.61237 LUMO: -0.48980 factor:1 | 1 (-1.35047) | -1 | -1 |
| G: -5278.76361 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.43270 HOMO: -6.80285 LUMO: -0.58232 factor:1 | 1 (-1.30340) | -1 | -1 |
| G: -5278.76361 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.35525 HOMO: -6.88992 LUMO: -0.70205 factor:1 | 1 (-1.22595) | -1 | -1 |
| G: -5278.76361 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.46111 HOMO: -6.95251 LUMO: -0.71838 factor:1 | 1 (-1.33181) | -1 | -1 |
| G: -5278.76361 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11545.03587 HOMO: -7.52123 LUMO: 0.27211 factor:1 | 1 (-1.90657) | -1 | -1 |
| G: -5278.76361 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.98261 HOMO: -6.76747 LUMO: -0.74015 factor:1 | 1 (-1.85331) | -1 | -1 |
| G: -5278.76361 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.90909 HOMO: -6.55250 LUMO: -0.49797 factor:1 | 1 (-1.77979) | -1 | -1 |
| G: -5278.76361 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.93578 HOMO: -6.50896 LUMO: -0.46804 factor:1 | 1 (-1.80648) | -1 | -1 |
| G: -5278.76361 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.82027 HOMO: -7.45320 LUMO: 0.08436 factor:1 | 1 (-1.69097) | -1 | -1 |
| G: -5278.76361 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.63080 HOMO: -6.82462 LUMO: -0.70477 factor:1 | 1 (-1.50150) | -1 | -1 |
| G: -5278.76361 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.81056 HOMO: -6.57155 LUMO: -0.43538 factor:1 | 1 (-1.68126) | -1 | -1 |
| G: -5278.76361 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.80862 HOMO: -6.72665 LUMO: -0.55239 factor:1 | 1 (-1.67932) | -1 | -1 |
| G: -5278.76361 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.93094 HOMO: -7.05319 LUMO: -1.08573 factor:1 | 1 (-1.80164) | -1 | -1 |
| G: -5278.76361 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.80364 HOMO: -6.56067 LUMO: -0.45715 factor:1 | 1 (-1.67434) | -1 | -1 |
| G: -5278.76361 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.81039 HOMO: -6.76475 LUMO: -0.53879 factor:1 | 1 (-1.68109) | -1 | -1 |
| G: -5278.76361 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.99143 HOMO: -6.67223 LUMO: -0.45987 factor:1 | 1 (-1.86213) | -1 | -1 |
| G: -5278.76361 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.76596 HOMO: -6.44094 LUMO: -0.72110 factor:1 | 1 (-1.63666) | -1 | -1 |
| G: -5278.76361 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.62051 HOMO: -6.66951 LUMO: -0.67756 factor:1 | 1 (-1.49121) | -1 | -1 |
| G: -5278.76361 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.66669 HOMO: -6.69400 LUMO: -0.62858 factor:1 | 1 (-1.53739) | -1 | -1 |
| G: -5278.76361 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11545.74132 HOMO: -6.51985 LUMO: -0.37007 factor:1 | 1 (-2.61202) | -1 | -1 |
| G: -5278.76361 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11546.37257 HOMO: -5.98378 LUMO: 0.78641 factor:1 | 1 (-3.24327) | -1 | -1 |
| G: -5278.76361 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11546.22590 HOMO: -6.11440 LUMO: 0.71294 factor:1 | 1 (-3.09660) | -1 | -1 |
| G: -5278.76361 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11545.48273 HOMO: -6.45182 LUMO: 0.63947 factor:1 | 1 (-2.35343) | -1 | -1 |
| G: -5278.76361 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11545.57745 HOMO: -6.78924 LUMO: 0.37007 factor:1 | 1 (-2.44815) | -1 | -1 |
| G: -5278.76361 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11545.72097 HOMO: -6.63686 LUMO: 0.54423 factor:1 | 1 (-2.59167) | -1 | -1 |
| G: -5278.76361 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.81973 HOMO: -6.66679 LUMO: 0.48708 factor:1 | 1 (-1.69043) | -1 | -1 |
| G: -5278.76361 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11545.02961 HOMO: -6.81917 LUMO: 0.31021 factor:1 | 1 (-1.90031) | -1 | -1 |
| G: -5278.76361 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.61711 HOMO: -6.28583 LUMO: 0.44899 factor:1 | 1 (-1.48781) | -1 | -1 |
| G: -5278.76361 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.91366 HOMO: -6.61237 LUMO: 0.49525 factor:1 | 1 (-1.78436) | -1 | -1 |
| G: -5278.76361 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.27909 HOMO: -7.08857 LUMO: 0.38368 factor:1 | 1 (-1.14979) | -1 | -1 |
| G: -5278.76361 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.40396 HOMO: -6.53890 LUMO: -0.68845 factor:1 | 1 (-1.27466) | -1 | -1 |
| G: -5278.76361 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.40916 HOMO: -6.56611 LUMO: -0.66396 factor:1 | 1 (-1.27986) | -1 | -1 |
| G: -5278.76361 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.26064 HOMO: -6.04909 LUMO: -0.59865 factor:1 | 1 (-1.13134) | -1 | -1 |
| G: -5278.76361 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.12722 HOMO: -6.74842 LUMO: -0.77825 factor:1 | 1 (-0.99792) | -1 | -1 |
| G: -5278.76361 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.01326 HOMO: -6.82462 LUMO: -0.61498 factor:1 | 1 (-0.88396) | -1 | -1 |
| G: -5278.76361 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.42505 HOMO: -7.40694 LUMO: 0.32926 factor:1 | 1 (-1.29575) | -1 | -1 |
| G: -5278.76361 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.40562 HOMO: -6.80557 LUMO: -0.57416 factor:1 | 1 (-1.27632) | -1 | -1 |
| G: -5278.76361 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.28739 HOMO: -6.76747 LUMO: -0.67484 factor:1 | 1 (-1.15809) | -1 | -1 |
| G: -5278.76361 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.18641 HOMO: -7.23279 LUMO: 0.48980 factor:1 | 1 (-1.05711) | -1 | -1 |
| G: -5278.76361 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.34173 HOMO: -6.62869 LUMO: -0.24762 factor:1 | 1 (-1.21243) | -1 | -1 |
| G: -5278.76361 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11545.17658 HOMO: -6.65863 LUMO: -0.28028 factor:1 | 1 (-2.04728) | -1 | -1 |
| G: -5278.76361 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11545.15511 HOMO: -6.50352 LUMO: -0.44899 factor:1 | 1 (-2.02581) | -1 | -1 |
| G: -5278.76361 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11545.32490 HOMO: -6.62053 LUMO: -0.88437 factor:1 | 1 (-2.19561) | -1 | -1 |
| G: -5278.76361 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11545.15067 HOMO: -6.73754 LUMO: -0.77825 factor:1 | 1 (-2.02137) | -1 | -1 |
| G: -5278.76361 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11545.23040 HOMO: -7.24639 LUMO: 0.35647 factor:1 | 1 (-2.10110) | -1 | -1 |
| G: -5278.76361 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.39370 HOMO: -6.46270 LUMO: -0.48164 factor:1 | 1 (-1.26440) | -1 | -1 |
| G: -5278.76361 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.52516 HOMO: -6.14161 LUMO: -0.66396 factor:1 | 1 (-1.39586) | -1 | -1 |
| G: -5278.76361 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.42641 HOMO: -6.63414 LUMO: 1.51295 factor:1 | 1 (-1.29711) | -1 | -1 |
| G: -5278.76361 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.36012 HOMO: -6.52529 LUMO: 1.65989 factor:1 | 1 (-1.23083) | -1 | -1 |
| G: -5278.76361 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.03160 HOMO: -6.63686 LUMO: 1.64629 factor:1 | 1 (-0.90230) | -1 | -1 |
| G: -5278.76361 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.98866 HOMO: -6.49808 LUMO: 1.60003 factor:1 | 1 (-0.85936) | -1 | -1 |
| G: -5278.76361 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.24840 HOMO: -6.85183 LUMO: 1.96194 factor:1 | 1 (-1.11910) | -1 | -1 |
| G: -5278.76361 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.57757 HOMO: -6.90081 LUMO: 1.82316 factor:1 | 1 (-1.44827) | -1 | -1 |
| G: -5278.76361 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.21038 HOMO: -6.20147 LUMO: 1.95106 factor:1 | 1 (-1.08108) | -1 | -1 |
| G: -5278.76361 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.17631 HOMO: -7.05047 LUMO: 1.94289 factor:1 | 1 (-1.04701) | -1 | -1 |
| G: -5278.76361 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.42404 HOMO: -6.11440 LUMO: 1.83949 factor:1 | 1 (-1.29474) | -1 | -1 |
| G: -5278.76361 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.96563 HOMO: -6.65046 LUMO: 1.59187 factor:1 | 1 (-1.83633) | -1 | -1 |
| G: -5278.76361 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.74794 HOMO: -6.81917 LUMO: 2.41365 factor:1 | 1 (-1.61864) | -1 | -1 |
| G: -5278.76361 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.61063 HOMO: -6.40284 LUMO: 2.48984 factor:1 | 1 (-1.48133) | -1 | -1 |
| G: -5278.76361 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.89850 HOMO: -7.04775 LUMO: 2.31025 factor:1 | 1 (-1.76920) | -1 | -1 |
| G: -5278.76361 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.68231 HOMO: -6.64774 LUMO: 2.20140 factor:1 | 1 (-1.55301) | -1 | -1 |
| G: -5278.76361 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.29708 HOMO: -6.72393 LUMO: 2.28304 factor:1 | 1 (-1.16778) | -1 | -1 |
| G: -5278.76361 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.72103 HOMO: -6.35114 LUMO: 1.84765 factor:1 | 1 (-1.59173) | -1 | -1 |
| G: -5278.76361 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.44946 HOMO: -6.41100 LUMO: 1.74697 factor:1 | 1 (-1.32016) | -1 | -1 |
| G: -5278.76361 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11546.19306 HOMO: -6.34297 LUMO: 1.55921 factor:1 | 1 (-3.06376) | -1 | -1 |
| G: -5278.76361 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11545.48572 HOMO: -6.31848 LUMO: 1.67622 factor:1 | 1 (-2.35642) | -1 | -1 |
| G: -5278.76361 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11545.60292 HOMO: -6.50896 LUMO: 2.02725 factor:1 | 1 (-2.47362) | -1 | -1 |
| G: -5278.76361 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11545.63136 HOMO: -6.28583 LUMO: 2.00548 factor:1 | 1 (-2.50206) | -1 | -1 |
| G: -5278.76361 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11545.50915 HOMO: -6.67495 LUMO: 1.92384 factor:1 | 1 (-2.37985) | -1 | -1 |
| G: -5278.76361 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11545.84630 HOMO: -6.17154 LUMO: 2.39732 factor:1 | 1 (-2.71700) | -1 | -1 |
| G: -5278.76361 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.66255 HOMO: -6.84911 LUMO: 2.24766 factor:1 | 1 (-1.53325) | -1 | -1 |
| G: -5278.76361 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.25925 HOMO: -6.77564 LUMO: 2.38372 factor:1 | 1 (-1.12995) | -1 | -1 |
| G: -5278.76361 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.25310 HOMO: -6.18243 LUMO: 2.40821 factor:1 | 1 (-1.12380) | -1 | -1 |
| G: -5278.76361 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.57790 HOMO: -6.40828 LUMO: 2.22589 factor:1 | 1 (-1.44860) | -1 | -1 |
| G: -5278.76361 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.46040 HOMO: -6.74570 LUMO: 1.88303 factor:1 | 1 (-1.33110) | -1 | -1 |
| G: -5278.76361 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.54301 HOMO: -6.29944 LUMO: 2.05174 factor:1 | 1 (-1.41371) | -1 | -1 |
| G: -5278.76361 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.67050 HOMO: -7.00693 LUMO: 2.16331 factor:1 | 1 (-1.54120) | -1 | -1 |
| G: -5278.76361 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.09696 HOMO: -6.89537 LUMO: 2.19596 factor:1 | 1 (-0.96766) | -1 | -1 |
| G: -5278.76361 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.71766 HOMO: -6.72665 LUMO: 2.03813 factor:1 | 1 (-0.58836) | -1 | -1 |
| G: -5278.76361 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.92989 HOMO: -6.69944 LUMO: 2.36467 factor:1 | 1 (-0.80059) | -1 | -1 |
| G: -5278.76361 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.00028 HOMO: -6.92802 LUMO: 1.72792 factor:1 | 1 (-0.87098) | -1 | -1 |
| G: -5278.76361 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.62618 HOMO: -6.12256 LUMO: 1.85310 factor:1 | 1 (-0.49688) | -1 | -1 |
| G: -5278.76361 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.09079 HOMO: -6.70489 LUMO: 2.20956 factor:1 | 1 (-0.96149) | -1 | -1 |
| G: -5278.76361 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.63655 HOMO: -6.94707 LUMO: 1.81500 factor:1 | 1 (-0.50725) | -1 | -1 |
| G: -5278.76361 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.57314 HOMO: -6.39468 LUMO: 1.79051 factor:1 | 1 (-0.44384) | -1 | -1 |
| G: -5278.76361 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.26525 HOMO: -6.69128 LUMO: 2.03813 factor:1 | 1 (-0.13595) | -1 | -1 |
| G: -5278.76361 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.05174 HOMO: -6.55250 LUMO: 2.00548 factor:1 | 1 (-0.92244) | -1 | -1 |
| G: -5278.76361 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.70844 HOMO: -6.24773 LUMO: 2.09256 factor:1 | 1 (-0.57914) | -1 | -1 |
| G: -5278.76361 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11546.11069 HOMO: -6.85727 LUMO: 1.70071 factor:1 | 1 (-2.98139) | -1 | -1 |
| G: -5278.76361 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11545.90505 HOMO: -6.71305 LUMO: 1.72520 factor:1 | 1 (-2.77575) | -1 | -1 |
| G: -5278.76361 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.97976 HOMO: -6.81101 LUMO: 2.15514 factor:1 | 1 (-1.85046) | -1 | -1 |
| G: -5278.76361 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11545.04120 HOMO: -6.93618 LUMO: 1.75513 factor:1 | 1 (-1.91190) | -1 | -1 |
| G: -5278.76361 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11545.10283 HOMO: -6.63686 LUMO: 2.09800 factor:1 | 1 (-1.97353) | -1 | -1 |
| G: -5278.76361 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11545.78606 HOMO: -6.98244 LUMO: 1.72520 factor:1 | 1 (-2.65676) | -1 | -1 |
| G: -5278.76361 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.59469 HOMO: -6.37019 LUMO: 2.35923 factor:1 | 1 (-1.46539) | -1 | -1 |
| G: -5278.76361 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11545.00370 HOMO: -6.55794 LUMO: 2.12521 factor:1 | 1 (-1.87440) | -1 | -1 |
| G: -5278.76361 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11545.17113 HOMO: -6.45998 LUMO: 1.93201 factor:1 | 1 (-2.04183) | -1 | -1 |
| G: -5278.76361 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.97189 HOMO: -6.71033 LUMO: 1.58370 factor:1 | 1 (-1.84259) | -1 | -1 |
| G: -5278.76361 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11545.76502 HOMO: -6.67223 LUMO: 1.52928 factor:1 | 1 (-2.63572) | -1 | -1 |
| G: -5278.76361 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.62386 HOMO: -6.72121 LUMO: 1.33608 factor:1 | 1 (-1.49456) | -1 | -1 |
| G: -5278.76361 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.79662 HOMO: -6.89264 LUMO: 2.08983 factor:1 | 1 (-1.66732) | -1 | -1 |
| G: -5278.76361 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.78743 HOMO: -6.31032 LUMO: 2.24766 factor:1 | 1 (-1.65813) | -1 | -1 |
| G: -5278.76361 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11545.69528 HOMO: -6.79740 LUMO: 2.09528 factor:1 | 1 (-2.56598) | -1 | -1 |
| G: -5278.76361 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.60655 HOMO: -6.78108 LUMO: 2.15786 factor:1 | 1 (-1.47725) | -1 | -1 |
| G: -5278.76361 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.89154 HOMO: -6.50896 LUMO: 2.15786 factor:1 | 1 (-1.76224) | -1 | -1 |
| G: -5278.76361 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11546.22729 HOMO: -6.56067 LUMO: 2.24494 factor:1 | 1 (-3.09799) | -1 | -1 |
| G: -5278.76361 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.86979 HOMO: -6.72938 LUMO: 2.24494 factor:1 | 1 (-1.74049) | -1 | -1 |
| G: -5278.76361 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11545.56853 HOMO: -6.40556 LUMO: 1.58642 factor:1 | 1 (-2.43923) | -1 | -1 |
| G: -5278.76361 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11545.61729 HOMO: -6.63141 LUMO: 1.66262 factor:1 | 1 (-2.48799) | -1 | -1 |
| G: -5278.76361 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.43564 HOMO: -6.97156 LUMO: 2.23678 factor:1 | 1 (-1.30634) | -1 | -1 |
| G: -5278.76361 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.78511 HOMO: -6.86271 LUMO: 1.91296 factor:1 | 1 (-1.65581) | -1 | -1 |
| G: -5278.76361 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11545.92037 HOMO: -6.50624 LUMO: 1.89119 factor:1 | 1 (-2.79107) | -1 | -1 |
| G: -5278.76361 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.73894 HOMO: -6.70761 LUMO: 1.56193 factor:1 | 1 (-0.60964) | -1 | -1 |
| G: -5278.76361 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.61864 HOMO: -6.60420 LUMO: 1.79595 factor:1 | 1 (-0.48934) | -1 | -1 |
| G: -5278.76361 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.60063 HOMO: -6.85727 LUMO: 2.26943 factor:1 | 1 (-0.47133) | -1 | -1 |
| G: -5278.76361 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.05247 HOMO: -6.23413 LUMO: 1.91024 factor:1 | 1 (-0.92317) | -1 | -1 |
| G: -5278.76361 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.87505 HOMO: -6.84366 LUMO: 2.01364 factor:1 | 1 (-0.74576) | -1 | -1 |
| G: -5278.76361 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.72836 HOMO: -6.63414 LUMO: 2.54971 factor:1 | 1 (-0.59906) | -1 | -1 |
| G: -5278.76361 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.63023 HOMO: -6.52257 LUMO: 2.42998 factor:1 | 1 (-0.50093) | -1 | -1 |
| G: -5278.76361 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11545.44172 HOMO: -6.61509 LUMO: 2.31297 factor:1 | 1 (-2.31242) | -1 | -1 |
| G: -5278.76361 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.58101 HOMO: -6.45998 LUMO: 2.23405 factor:1 | 1 (-0.45171) | -1 | -1 |
| G: -5278.76361 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.66384 HOMO: -6.86271 LUMO: 2.22317 factor:1 | 1 (-0.53454) | -1 | -1 |
| G: -5278.76361 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.48816 HOMO: -6.84366 LUMO: 2.11432 factor:1 | 1 (-0.35886) | -1 | -1 |
| G: -5278.76361 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.75369 HOMO: -6.85999 LUMO: 2.44902 factor:1 | 1 (-0.62439) | -1 | -1 |
| G: -5278.76361 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.47015 HOMO: -6.73482 LUMO: 1.93745 factor:1 | 1 (-0.34085) | -1 | -1 |
| G: -5278.76361 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.33687 HOMO: -6.91441 LUMO: 2.32385 factor:1 | 1 (-0.20757) | -1 | -1 |
| G: -5278.76361 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.39510 HOMO: -6.16066 LUMO: 2.26399 factor:1 | 1 (-0.26580) | -1 | -1 |
| G: -5278.76361 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.15093 HOMO: -6.71305 LUMO: 2.38644 factor:1 | 1 (-0.02163) | -1 | -1 |
| G: -5278.76361 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.76964 HOMO: -7.08312 LUMO: 2.01636 factor:1 | 1 (-0.64034) | 1 | 1 |
| G: -5278.76361 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.97427 HOMO: -6.15249 LUMO: 1.90752 factor:1 | 1 (-0.84497) | -1 | -1 |
| G: -5278.76361 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.71309 HOMO: -6.83006 LUMO: 2.25855 factor:1 | 1 (-0.58379) | -1 | -1 |
| G: -5278.76361 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.88624 HOMO: -6.77836 LUMO: 2.24766 factor:1 | 1 (-0.75694) | -1 | -1 |
| G: -5278.76361 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.61170 HOMO: -6.66951 LUMO: 2.35923 factor:1 | 1 (-0.48240) | -1 | -1 |
| G: -5278.76361 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.57162 HOMO: -6.68312 LUMO: 2.30208 factor:1 | 1 (-0.44232) | -1 | -1 |
| G: -5278.76361 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11545.62077 HOMO: -6.49808 LUMO: 2.49801 factor:1 | 1 (-2.49147) | -1 | -1 |
| G: -5278.76361 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.64289 HOMO: -6.62325 LUMO: 1.89935 factor:1 | 1 (-0.51359) | -1 | -1 |
| G: -5278.76361 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.57510 HOMO: -6.80829 LUMO: 1.91296 factor:1 | 1 (-0.44580) | -1 | -1 |
| G: -5278.76361 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.73206 HOMO: -6.64230 LUMO: 2.13065 factor:1 | 1 (-0.60276) | -1 | -1 |
| G: -5278.76361 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.67094 HOMO: -6.40556 LUMO: 1.83949 factor:1 | 1 (-0.54164) | -1 | -1 |
| G: -5278.76361 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.43638 HOMO: -6.48175 LUMO: 1.72248 factor:1 | 1 (-0.30708) | -1 | -1 |
| G: -5278.76361 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.51186 HOMO: -6.61781 LUMO: 2.11432 factor:1 | 1 (-0.38256) | -1 | -1 |
| G: -5278.76361 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.04518 HOMO: -6.34570 LUMO: 2.22317 factor:1 | 1 (-0.91588) | -1 | -1 |
| G: -5278.76361 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.91555 HOMO: -7.00149 LUMO: 1.80139 factor:1 | 1 (-0.78625) | -1 | -1 |
| G: -5278.76361 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.42993 HOMO: -6.66951 LUMO: 2.13065 factor:1 | 1 (-0.30063) | -1 | -1 |
| G: -5278.76361 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.20416 HOMO: -6.54434 LUMO: 2.20140 factor:1 | 1 (-0.07486) | -1 | -1 |
| G: -5278.76361 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.51331 HOMO: -6.67767 LUMO: 2.02997 factor:1 | 1 (-0.38401) | -1 | -1 |
| G: -5278.76361 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.73535 HOMO: -6.49536 LUMO: 2.42998 factor:1 | 1 (-0.60605) | -1 | -1 |
| G: -5278.76361 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11545.86037 HOMO: -6.70761 LUMO: 2.71025 factor:1 | 1 (-2.73107) | -1 | -1 |
| G: -5278.76361 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.46894 HOMO: -6.62869 LUMO: 2.11160 factor:1 | 1 (-1.33964) | -1 | -1 |
| G: -5278.76361 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.42519 HOMO: -6.61781 LUMO: 2.24494 factor:1 | 1 (-1.29589) | -1 | -1 |
| G: -5278.76361 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.26820 HOMO: -6.66135 LUMO: 2.20956 factor:1 | 1 (-1.13891) | -1 | -1 |
| G: -5278.76361 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.46824 HOMO: -6.95523 LUMO: 2.03813 factor:1 | 1 (-1.33894) | -1 | -1 |
| G: -5278.76361 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.93647 HOMO: -7.11578 LUMO: 2.41365 factor:1 | 1 (-0.80717) | 1 | 1 |
| G: -5278.76361 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.84099 HOMO: -6.99061 LUMO: 2.13881 factor:1 | 1 (-0.71169) | -1 | -1 |
| G: -5278.76361 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.73366 HOMO: -6.43277 LUMO: 2.01364 factor:1 | 1 (-0.60436) | -1 | -1 |
| G: -5278.76361 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.79252 HOMO: -6.79196 LUMO: 2.04358 factor:1 | 1 (-0.66322) | -1 | -1 |
| G: -5278.76361 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.44541 HOMO: -7.08584 LUMO: 1.99732 factor:1 | 1 (-0.31611) | 1 | 1 |
| G: -5278.76361 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.64417 HOMO: -6.46815 LUMO: 2.29936 factor:1 | 1 (-0.51487) | -1 | -1 |
| G: -5278.76361 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.43045 HOMO: -6.78108 LUMO: 1.93745 factor:1 | 1 (-0.30115) | -1 | -1 |
| G: -5278.76361 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.21994 HOMO: -6.43277 LUMO: 1.80956 factor:1 | 1 (-0.09064) | -1 | -1 |
| G: -5278.76361 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.33649 HOMO: -6.71577 LUMO: -0.81090 factor:1 | 1 (-0.20719) | -1 | -1 |
| G: -5278.76361 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.56172 HOMO: -7.14027 LUMO: -0.68028 factor:1 | 1 (-0.43242) | -1 | -1 |
| G: -5278.76361 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11545.47721 HOMO: -7.03414 LUMO: -0.69661 factor:1 | 1 (-2.34791) | -1 | -1 |
| G: -5278.76361 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.51663 HOMO: -6.64502 LUMO: -0.47348 factor:1 | 1 (-0.38733) | -1 | -1 |
| G: -5278.76361 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.21259 HOMO: -6.60692 LUMO: 2.12793 factor:1 | 1 (-0.08329) | -1 | -1 |
| G: -5278.76361 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.33396 HOMO: -6.66407 LUMO: 1.94561 factor:1 | 1 (-0.20466) | -1 | -1 |
| G: -5278.76361 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.08609 HOMO: -7.10217 LUMO: 1.92384 factor:1 | -1 (0.04321) | 1 | 1 |
| G: -5278.76361 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.55102 HOMO: -6.84094 LUMO: 1.66534 factor:1 | 1 (-0.42172) | -1 | -1 |
| G: -5278.76361 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11542.52053 HOMO: -6.93618 LUMO: 2.13065 factor:1 | -1 (0.60877) | -1 | -1 |
| G: -5278.76361 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11542.92652 HOMO: -6.60692 LUMO: 2.20684 factor:1 | -1 (0.20278) | -1 | -1 |
| G: -5278.76361 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11542.69011 HOMO: -6.85727 LUMO: 2.19324 factor:1 | -1 (0.43919) | -1 | -1 |
| G: -5278.76361 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11542.32251 HOMO: -6.31032 LUMO: 1.76330 factor:1 | -1 (0.80679) | -1 | -1 |
| G: -5278.76361 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11542.69849 HOMO: -6.43821 LUMO: 2.10072 factor:1 | -1 (0.43081) | -1 | -1 |
| G: -5278.76361 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11542.96902 HOMO: -6.42189 LUMO: 2.19596 factor:1 | -1 (0.16028) | -1 | -1 |
| G: -5278.76361 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.26408 HOMO: -6.40556 LUMO: 2.02181 factor:1 | 1 (-0.13478) | -1 | -1 |
| G: -5278.76361 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.37118 HOMO: -6.41372 LUMO: 2.26671 factor:1 | 1 (-0.24188) | -1 | -1 |
| G: -5278.76361 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.31360 HOMO: -6.60692 LUMO: 2.09800 factor:1 | 1 (-0.18430) | -1 | -1 |
| G: -5278.76361 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.08467 HOMO: -6.75931 LUMO: 1.76602 factor:1 | -1 (0.04463) | -1 | -1 |
| G: -5278.76361 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.35915 HOMO: -6.39195 LUMO: 1.84221 factor:1 | 1 (-0.22985) | -1 | -1 |
| G: -5278.76361 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.48675 HOMO: -6.74570 LUMO: 2.04085 factor:1 | 1 (-0.35745) | -1 | -1 |
| G: -5278.76361 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.93766 HOMO: -6.77019 LUMO: 2.16875 factor:1 | 1 (-1.80836) | -1 | -1 |
| G: -5278.76361 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11546.05529 HOMO: -6.15522 LUMO: 1.81772 factor:1 | 1 (-2.92599) | -1 | -1 |
| G: -5278.76361 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11545.13747 HOMO: -6.48175 LUMO: 2.02453 factor:1 | 1 (-2.00817) | -1 | -1 |
| G: -5278.76361 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11545.01069 HOMO: -6.57427 LUMO: 1.77962 factor:1 | 1 (-1.88140) | -1 | -1 |
| G: -5278.76361 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.82775 HOMO: -6.57699 LUMO: 2.42998 factor:1 | 1 (-1.69845) | -1 | -1 |
| G: -5278.76361 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.64329 HOMO: -6.35386 LUMO: 2.25310 factor:1 | 1 (-1.51399) | -1 | -1 |
| G: -5278.76361 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.75387 HOMO: -6.80013 LUMO: 2.11160 factor:1 | 1 (-1.62457) | -1 | -1 |
| G: -5278.76361 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.78204 HOMO: -6.24229 LUMO: 2.05718 factor:1 | 1 (-1.65274) | -1 | -1 |
| G: -5278.76361 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.69504 HOMO: -6.42733 LUMO: 1.76874 factor:1 | 1 (-1.56574) | -1 | -1 |
| G: -5278.76361 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.48829 HOMO: -6.56883 LUMO: 2.36195 factor:1 | 1 (-1.35899) | -1 | -1 |
| G: -5278.76361 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.48917 HOMO: -6.72665 LUMO: 2.28848 factor:1 | 1 (-0.35987) | -1 | -1 |
| G: -5278.76361 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.47815 HOMO: -6.39195 LUMO: 1.79051 factor:1 | 1 (-0.34885) | -1 | -1 |
| G: -5278.76361 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.68751 HOMO: -6.70761 LUMO: 0.15510 factor:1 | 1 (-0.55821) | -1 | -1 |
| G: -5278.76361 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.50016 HOMO: -6.44366 LUMO: -0.16871 factor:1 | 1 (-0.37086) | -1 | -1 |
| G: -5278.76361 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.35880 HOMO: -6.68584 LUMO: 1.69527 factor:1 | 1 (-0.22950) | -1 | -1 |
| G: -5278.76361 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.28590 HOMO: -6.26950 LUMO: 1.61636 factor:1 | 1 (-0.15660) | -1 | -1 |
| G: -5278.76361 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.50318 HOMO: -6.47631 LUMO: 1.98915 factor:1 | 1 (-0.37388) | -1 | -1 |
| G: -5278.76361 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.58950 HOMO: -6.58243 LUMO: 1.97283 factor:1 | 1 (-0.46020) | -1 | -1 |
| G: -5278.76361 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.76117 HOMO: -6.51713 LUMO: 1.97283 factor:1 | 1 (-1.63187) | -1 | -1 |
| G: -5278.76361 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.88120 HOMO: -6.65046 LUMO: 1.69255 factor:1 | 1 (-1.75190) | -1 | -1 |
| G: -5278.76361 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.97758 HOMO: -6.26406 LUMO: 2.21773 factor:1 | 1 (-1.84828) | -1 | -1 |
| G: -5278.76361 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11545.81251 HOMO: -6.88992 LUMO: 2.28304 factor:1 | 1 (-2.68321) | -1 | -1 |
| G: -5278.76361 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11545.03987 HOMO: -6.67767 LUMO: 2.34834 factor:1 | 1 (-1.91057) | -1 | -1 |
| G: -5278.76361 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11545.14645 HOMO: -6.52801 LUMO: 2.10344 factor:1 | 1 (-2.01715) | -1 | -1 |
| G: -5278.76361 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.94811 HOMO: -6.52801 LUMO: 2.24222 factor:1 | 1 (-1.81881) | -1 | -1 |
| G: -5278.76361 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.75036 HOMO: -6.17154 LUMO: 1.89663 factor:1 | 1 (-1.62106) | -1 | -1 |
| G: -5278.76361 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.75257 HOMO: -6.42733 LUMO: 2.15514 factor:1 | 1 (-1.62327) | -1 | -1 |
| G: -5278.76361 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.97088 HOMO: -6.36474 LUMO: 2.01364 factor:1 | 1 (-1.84158) | -1 | -1 |
| G: -5278.76361 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.60236 HOMO: -6.82189 LUMO: 1.86942 factor:1 | 1 (-1.47306) | -1 | -1 |
| G: -5278.76361 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.76081 HOMO: -6.60148 LUMO: 2.00548 factor:1 | 1 (-1.63151) | -1 | -1 |
| G: -5278.76361 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.88860 HOMO: -6.67767 LUMO: 2.15786 factor:1 | 1 (-1.75930) | -1 | -1 |
| G: -5278.76361 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.89880 HOMO: -6.79196 LUMO: 2.06534 factor:1 | 1 (-1.76950) | -1 | -1 |
| G: -5278.76361 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11545.01695 HOMO: -6.70216 LUMO: 1.83405 factor:1 | 1 (-1.88765) | -1 | -1 |
| G: -5278.76361 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.92128 HOMO: -6.58788 LUMO: 1.79051 factor:1 | 1 (-1.79198) | -1 | -1 |
| G: -5278.76361 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.77352 HOMO: -6.34842 LUMO: 1.80139 factor:1 | 1 (-1.64422) | -1 | -1 |
| G: -5278.76361 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.61442 HOMO: -6.48175 LUMO: 1.95922 factor:1 | 1 (-0.48512) | -1 | -1 |
| G: -5278.76361 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.38076 HOMO: -6.71033 LUMO: 2.02997 factor:1 | 1 (-0.25146) | -1 | -1 |
| G: -5278.76361 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.34337 HOMO: -6.89264 LUMO: 2.42726 factor:1 | 1 (-0.21407) | -1 | -1 |
| G: -5278.76361 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.42792 HOMO: -6.74570 LUMO: 2.20684 factor:1 | 1 (-0.29862) | -1 | -1 |
| G: -5278.76361 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.40253 HOMO: -6.30216 LUMO: 2.15242 factor:1 | 1 (-0.27323) | -1 | -1 |
| G: -5278.76361 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.61347 HOMO: -6.94979 LUMO: 2.43814 factor:1 | 1 (-0.48417) | -1 | -1 |
| G: -5278.76361 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.71918 HOMO: -6.97972 LUMO: 2.11432 factor:1 | 1 (-1.58988) | -1 | -1 |
| G: -5278.76361 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.79064 HOMO: -6.17154 LUMO: 1.98099 factor:1 | 1 (-1.66134) | -1 | -1 |
| G: -5278.76361 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.88634 HOMO: -6.74026 LUMO: 2.21501 factor:1 | 1 (-1.75704) | -1 | -1 |
| G: -5278.76361 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.68715 HOMO: -6.72393 LUMO: 2.19596 factor:1 | 1 (-1.55785) | -1 | -1 |
| G: -5278.76361 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.53357 HOMO: -6.11440 LUMO: 2.10072 factor:1 | 1 (-1.40427) | -1 | -1 |
| G: -5278.76361 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11545.20196 HOMO: -6.34297 LUMO: 1.92657 factor:1 | 1 (-2.07266) | -1 | -1 |
| G: -5278.76361 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.63232 HOMO: -6.24773 LUMO: 2.00276 factor:1 | 1 (-1.50302) | -1 | -1 |
| G: -5278.76361 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.50492 HOMO: -6.75114 LUMO: 1.98643 factor:1 | 1 (-1.37562) | -1 | -1 |
| G: -5278.76361 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.33490 HOMO: -6.69128 LUMO: 2.08711 factor:1 | 1 (-1.20560) | -1 | -1 |
| G: -5278.76361 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.49586 HOMO: -6.65318 LUMO: 2.15514 factor:1 | 1 (-1.36656) | -1 | -1 |
| G: -5278.76361 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.69700 HOMO: -6.67495 LUMO: 1.72248 factor:1 | 1 (-1.56770) | -1 | -1 |
| G: -5278.76361 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.50557 HOMO: -6.58243 LUMO: 1.83405 factor:1 | 1 (-1.37627) | -1 | -1 |
| G: -5278.76361 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.56146 HOMO: -6.61237 LUMO: 1.69799 factor:1 | 1 (-1.43216) | -1 | -1 |
| G: -5278.76361 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.40549 HOMO: -6.57427 LUMO: 2.29936 factor:1 | 1 (-1.27619) | -1 | -1 |
| G: -5278.76361 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.57651 HOMO: -6.40012 LUMO: 2.35378 factor:1 | 1 (-1.44721) | -1 | -1 |
| G: -5278.76361 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.12867 HOMO: -6.90081 LUMO: 2.26671 factor:1 | -1 (0.00063) | -1 | -1 |
| G: -5278.76361 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.32451 HOMO: -6.44910 LUMO: 2.25855 factor:1 | 1 (-0.19521) | -1 | -1 |
| G: -5278.76361 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11542.84540 HOMO: -6.61509 LUMO: 2.26943 factor:1 | -1 (0.28390) | -1 | -1 |
| G: -5278.76361 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.10288 HOMO: -6.78924 LUMO: 2.09256 factor:1 | -1 (0.02642) | -1 | -1 |
| G: -5278.76361 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.31758 HOMO: -6.47087 LUMO: 1.97555 factor:1 | 1 (-0.18828) | -1 | -1 |
| G: -5278.76361 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11542.84924 HOMO: -6.75931 LUMO: 1.98643 factor:1 | -1 (0.28006) | -1 | -1 |
| G: -5278.76361 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.16522 HOMO: -6.17971 LUMO: 2.09800 factor:1 | 1 (-0.03592) | -1 | -1 |
| G: -5278.76361 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.21412 HOMO: -6.83006 LUMO: 1.91840 factor:1 | 1 (-0.08482) | -1 | -1 |
| G: -5278.76361 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11542.92222 HOMO: -6.72938 LUMO: 2.17419 factor:1 | -1 (0.20708) | -1 | -1 |
| G: -5278.76361 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11542.61759 HOMO: -6.78924 LUMO: 2.42726 factor:1 | -1 (0.51171) | -1 | -1 |
| G: -5278.76361 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.13836 HOMO: -6.41372 LUMO: 1.93745 factor:1 | 1 (-0.00906) | -1 | -1 |
| G: -5278.76361 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.92281 HOMO: -6.85455 LUMO: 2.14970 factor:1 | 1 (-0.79351) | -1 | -1 |
| G: -5278.76361 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.81467 HOMO: -6.38651 LUMO: 2.18507 factor:1 | 1 (-0.68537) | -1 | -1 |
| G: -5278.76361 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.73241 HOMO: -6.81373 LUMO: 2.00548 factor:1 | 1 (-0.60311) | -1 | -1 |
| G: -5278.76361 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.91141 HOMO: -6.64774 LUMO: 2.41365 factor:1 | 1 (-0.78211) | -1 | -1 |
| G: -5278.76361 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.05291 HOMO: -6.70489 LUMO: 2.31569 factor:1 | 1 (-0.92361) | -1 | -1 |
| G: -5278.76361 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.91933 HOMO: -6.49264 LUMO: 1.78779 factor:1 | 1 (-0.79003) | -1 | -1 |
| G: -5278.76361 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.15833 HOMO: -6.81101 LUMO: 1.86670 factor:1 | 1 (-1.02903) | -1 | -1 |
| G: -5278.76361 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.58455 HOMO: -6.72121 LUMO: 1.48846 factor:1 | 1 (-0.45525) | -1 | -1 |
| G: -5278.76361 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.59551 HOMO: -6.35930 LUMO: 1.78507 factor:1 | 1 (-0.46621) | -1 | -1 |
| G: -5278.76361 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.94265 HOMO: -6.38651 LUMO: 2.04358 factor:1 | 1 (-0.81335) | -1 | -1 |
| G: -5278.76361 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.62400 HOMO: -6.42189 LUMO: 1.99187 factor:1 | 1 (-0.49470) | -1 | -1 |
| G: -5278.76361 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.50269 HOMO: -6.69400 LUMO: 1.61091 factor:1 | 1 (-0.37339) | -1 | -1 |
| G: -5278.76361 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.63921 HOMO: -6.81101 LUMO: 2.17419 factor:1 | 1 (-0.50991) | -1 | -1 |
| G: -5278.76361 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.32756 HOMO: -6.90897 LUMO: 2.28576 factor:1 | 1 (-0.19826) | -1 | -1 |
| G: -5278.76361 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.36250 HOMO: -6.75387 LUMO: 2.31297 factor:1 | 1 (-0.23320) | -1 | -1 |
| G: -5278.76361 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.53415 HOMO: -7.05863 LUMO: 2.18780 factor:1 | 1 (-0.40485) | -1 | -1 |
| G: -5278.76361 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.69010 HOMO: -6.56611 LUMO: 1.99187 factor:1 | 1 (-0.56080) | -1 | -1 |
| G: -5278.76361 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.73818 HOMO: -6.59060 LUMO: 1.86398 factor:1 | 1 (-0.60888) | -1 | -1 |
| G: -5278.76361 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.75481 HOMO: -6.59060 LUMO: 1.59459 factor:1 | 1 (-0.62551) | -1 | -1 |
| G: -5278.76361 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.62490 HOMO: -6.57699 LUMO: 1.48030 factor:1 | 1 (-0.49560) | -1 | -1 |
| G: -5278.76361 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.92477 HOMO: -6.99605 LUMO: 2.30208 factor:1 | 1 (-0.79547) | -1 | -1 |
| G: -5278.76361 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.64471 HOMO: -6.42189 LUMO: 2.20412 factor:1 | 1 (-0.51541) | -1 | -1 |
| G: -5278.76361 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.50095 HOMO: -7.15115 LUMO: 1.83405 factor:1 | 1 (-0.37165) | 1 | 1 |
| G: -5278.76361 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.36065 HOMO: -7.08040 LUMO: 2.21773 factor:1 | 1 (-0.23135) | 1 | 1 |
| G: -5278.76361 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.51331 HOMO: -6.72121 LUMO: 1.89663 factor:1 | 1 (-0.38401) | -1 | -1 |
| G: -5278.76361 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.70166 HOMO: -6.25590 LUMO: 1.85037 factor:1 | 1 (-0.57236) | -1 | -1 |
| G: -5278.76361 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.74594 HOMO: -6.70489 LUMO: 1.98915 factor:1 | 1 (-0.61664) | -1 | -1 |
| G: -5278.76361 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.50060 HOMO: -6.53617 LUMO: 2.08439 factor:1 | 1 (-0.37130) | -1 | -1 |
| G: -5278.76361 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.94047 HOMO: -6.69944 LUMO: 1.98915 factor:1 | 1 (-0.81117) | -1 | -1 |
| G: -5278.76361 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.67739 HOMO: -6.79468 LUMO: 1.96466 factor:1 | 1 (-0.54809) | -1 | -1 |
| G: -5278.76361 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.41690 HOMO: -6.79468 LUMO: 1.99459 factor:1 | 1 (-0.28760) | -1 | -1 |
| G: -5278.76361 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.54735 HOMO: -6.58788 LUMO: 1.98371 factor:1 | 1 (-0.41805) | -1 | -1 |
| G: -5278.76361 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.30215 HOMO: -6.58788 LUMO: 2.16603 factor:1 | 1 (-0.17285) | -1 | -1 |
| G: -5278.76361 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.50544 HOMO: -6.56883 LUMO: 1.64085 factor:1 | 1 (-0.37614) | -1 | -1 |
| G: -5278.76361 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.72428 HOMO: -7.19197 LUMO: 2.66127 factor:1 | 1 (-0.59498) | 1 | 1 |
| G: -5278.76361 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.25757 HOMO: -6.48175 LUMO: 2.40004 factor:1 | 1 (-1.12827) | -1 | -1 |
| G: -5278.76361 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.50209 HOMO: -6.18515 LUMO: 2.27759 factor:1 | 1 (-1.37279) | -1 | -1 |
| G: -5278.76361 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.25318 HOMO: -6.64774 LUMO: 2.13337 factor:1 | 1 (-1.12388) | -1 | -1 |
| G: -5278.76361 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.14853 HOMO: -6.39740 LUMO: 1.95106 factor:1 | 1 (-1.01923) | -1 | -1 |
| G: -5278.76361 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.09802 HOMO: -6.59332 LUMO: 1.81772 factor:1 | 1 (-0.96873) | -1 | -1 |
| G: -5278.76361 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.15144 HOMO: -6.68312 LUMO: 2.41909 factor:1 | 1 (-1.02214) | -1 | -1 |
| G: -5278.76361 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.02801 HOMO: -5.87494 LUMO: 2.18235 factor:1 | 1 (-0.89871) | -1 | -1 |
| G: -5278.76361 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.42717 HOMO: -6.30488 LUMO: 2.04902 factor:1 | 1 (-1.29787) | -1 | -1 |
| G: -5278.76361 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.33482 HOMO: -6.65046 LUMO: 2.05446 factor:1 | 1 (-1.20552) | -1 | -1 |
| G: -5278.76361 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.34568 HOMO: -6.55794 LUMO: 2.06807 factor:1 | 1 (-1.21638) | -1 | -1 |
| G: -5278.76361 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.21884 HOMO: -6.68040 LUMO: 1.99187 factor:1 | 1 (-1.08954) | -1 | -1 |
| G: -5278.76361 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.66922 HOMO: -6.60965 LUMO: 2.18780 factor:1 | 1 (-1.53992) | -1 | -1 |
| G: -5278.76361 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.51431 HOMO: -6.88176 LUMO: 2.10344 factor:1 | 1 (-0.38501) | -1 | -1 |
| G: -5278.76361 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.38381 HOMO: -6.63414 LUMO: 1.70615 factor:1 | 1 (-0.25451) | -1 | -1 |
| G: -5278.76361 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.48131 HOMO: -7.15115 LUMO: 2.07351 factor:1 | 1 (-0.35201) | 1 | 1 |
| G: -5278.76361 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.60708 HOMO: -6.85727 LUMO: 2.27759 factor:1 | 1 (-0.47778) | -1 | -1 |
| G: -5278.76361 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.60996 HOMO: -6.91713 LUMO: 2.28848 factor:1 | 1 (-0.48066) | -1 | -1 |
| G: -5278.76361 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.29692 HOMO: -7.10217 LUMO: 2.14698 factor:1 | 1 (-0.16762) | 1 | 1 |
| G: -5278.76361 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.44560 HOMO: -6.78108 LUMO: 2.45447 factor:1 | 1 (-0.31631) | -1 | -1 |
| G: -5278.76361 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.17872 HOMO: -6.78380 LUMO: 2.43542 factor:1 | 1 (-0.04942) | -1 | -1 |
| G: -5278.76361 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.23605 HOMO: -6.60965 LUMO: 2.33474 factor:1 | 1 (-0.10675) | -1 | -1 |
| G: -5278.76361 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.63940 HOMO: -6.72665 LUMO: 2.25855 factor:1 | 1 (-0.51010) | -1 | -1 |
| G: -5278.76361 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.70509 HOMO: -6.27495 LUMO: 2.04358 factor:1 | 1 (-0.57579) | -1 | -1 |
| G: -5278.76361 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.60539 HOMO: -6.17426 LUMO: 1.45853 factor:1 | 1 (-0.47609) | -1 | -1 |
| G: -5278.76361 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.49973 HOMO: -7.21374 LUMO: 2.33474 factor:1 | 1 (-0.37043) | 1 | 1 |
| G: -5278.76361 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.40384 HOMO: -6.94707 LUMO: 1.81772 factor:1 | 1 (-0.27454) | -1 | -1 |
| G: -5278.76361 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.71677 HOMO: -6.80829 LUMO: 0.17960 factor:1 | 1 (-0.58747) | -1 | -1 |
| G: -5278.76361 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.59089 HOMO: -7.19469 LUMO: 1.60819 factor:1 | 1 (-0.46159) | 1 | 1 |
| G: -5278.76361 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.88830 HOMO: -6.78652 LUMO: 0.53334 factor:1 | 1 (-1.75900) | -1 | -1 |
| G: -5278.76361 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.64190 HOMO: -6.70489 LUMO: 0.74559 factor:1 | 1 (-1.51260) | -1 | -1 |
| G: -5278.76361 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.86288 HOMO: -6.72393 LUMO: 0.88981 factor:1 | 1 (-1.73358) | -1 | -1 |
| G: -5278.76361 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.62693 HOMO: -4.54430 LUMO: -0.90614 factor:1 | 1 (-1.49763) | -1 | -1 |
| G: -5278.76361 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.73061 HOMO: -6.83006 LUMO: 0.47348 factor:1 | 1 (-1.60131) | -1 | -1 |
| G: -5278.76361 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.96188 HOMO: -7.07496 LUMO: 0.50613 factor:1 | 1 (-1.83258) | -1 | -1 |
| G: -5278.76361 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.72274 HOMO: -6.62053 LUMO: 0.74559 factor:1 | 1 (-1.59344) | -1 | -1 |
| G: -5278.76361 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.94370 HOMO: -6.79196 LUMO: 1.80139 factor:1 | 1 (-1.81440) | -1 | -1 |
| G: -5278.76361 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.81124 HOMO: -6.71033 LUMO: 0.40817 factor:1 | 1 (-1.68194) | -1 | -1 |
| G: -5278.76361 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.74065 HOMO: -6.74026 LUMO: 0.95784 factor:1 | 1 (-1.61135) | -1 | -1 |
| G: -5278.76361 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.61461 HOMO: -7.34707 LUMO: 0.40001 factor:1 | 1 (-1.48531) | -1 | -1 |
| G: -5278.76361 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.91652 HOMO: -6.19875 LUMO: -0.88709 factor:1 | 1 (-1.78722) | -1 | -1 |
| G: -5278.76361 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.52432 HOMO: -6.48719 LUMO: -0.14694 factor:1 | 1 (-1.39502) | -1 | -1 |
| G: -5278.76361 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.55284 HOMO: -6.73482 LUMO: -0.01633 factor:1 | 1 (-1.42354) | -1 | -1 |
| G: -5278.76361 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.75469 HOMO: -7.05591 LUMO: -0.20136 factor:1 | 1 (-1.62539) | -1 | -1 |
| G: -5278.76361 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.75216 HOMO: -6.38651 LUMO: -2.07895 factor:1 | 1 (-1.62286) | -1 | -1 |
| G: -5278.76361 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.57123 HOMO: -6.85455 LUMO: -1.03403 factor:1 | 1 (-1.44193) | -1 | -1 |
| G: -5278.76361 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.67197 HOMO: -6.72121 LUMO: -0.99322 factor:1 | 1 (-1.54267) | -1 | -1 |
| G: -5278.76361 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.58407 HOMO: -6.53890 LUMO: -0.10885 factor:1 | 1 (-1.45478) | -1 | -1 |
| G: -5278.76361 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.34249 HOMO: -6.68312 LUMO: 0.21225 factor:1 | 1 (-1.21319) | -1 | -1 |
| G: -5278.76361 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.96882 HOMO: -6.68040 LUMO: 0.21225 factor:1 | 1 (-1.83952) | -1 | -1 |
| G: -5278.76361 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11545.95071 HOMO: -6.76475 LUMO: -0.64491 factor:1 | 1 (-2.82141) | -1 | -1 |
| G: -5278.76361 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11545.06378 HOMO: -6.48175 LUMO: 0.41633 factor:1 | 1 (-1.93448) | -1 | -1 |
| G: -5278.76361 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.90569 HOMO: -6.42733 LUMO: 0.16599 factor:1 | 1 (-1.77639) | -1 | -1 |
| G: -5278.76361 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.68772 HOMO: -6.66679 LUMO: 0.77825 factor:1 | 1 (-1.55842) | -1 | -1 |
| G: -5278.76361 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.33586 HOMO: -6.75931 LUMO: -0.73471 factor:1 | 1 (-0.20656) | -1 | -1 |
| G: -5278.76361 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.67075 HOMO: -6.53617 LUMO: 0.38096 factor:1 | 1 (-0.54145) | -1 | -1 |
| G: -5278.76361 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.35251 HOMO: -6.34297 LUMO: 0.35375 factor:1 | 1 (-0.22321) | -1 | -1 |
| G: -5278.76361 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.35733 HOMO: -7.11850 LUMO: -0.03265 factor:1 | 1 (-0.22803) | -1 | -1 |
| G: -5278.76361 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.12935 HOMO: -5.21914 LUMO: 1.29798 factor:1 | 1 (-0.00005) | -1 | -1 |
| G: -5278.76361 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.54468 HOMO: -7.09129 LUMO: -0.66668 factor:1 | 1 (-0.41538) | -1 | -1 |
| G: -5278.76361 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11542.89691 HOMO: -6.96884 LUMO: -0.31021 factor:1 | -1 (0.23239) | -1 | -1 |
| G: -5278.76361 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11542.95327 HOMO: -6.51713 LUMO: -0.59865 factor:1 | -1 (0.17603) | -1 | -1 |
| G: -5278.76361 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.28767 HOMO: -6.69400 LUMO: -0.07075 factor:1 | 1 (-0.15837) | -1 | -1 |
| G: -5278.76361 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11542.61947 HOMO: -5.28173 LUMO: 1.17281 factor:1 | -1 (0.50983) | -1 | -1 |
| G: -5278.76361 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11542.93324 HOMO: -6.54434 LUMO: 0.32109 factor:1 | -1 (0.19606) | -1 | -1 |
| G: -5278.76361 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.14171 HOMO: -6.79740 LUMO: -0.24762 factor:1 | 1 (-0.01241) | -1 | -1 |
| G: -5278.76361 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11542.60072 HOMO: -6.91986 LUMO: -0.14694 factor:1 | -1 (0.52858) | -1 | -1 |
| G: -5278.76361 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11542.79128 HOMO: -6.75114 LUMO: 0.18504 factor:1 | -1 (0.33802) | -1 | -1 |
| G: -5278.76361 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.05811 HOMO: -6.74842 LUMO: 0.69389 factor:1 | -1 (0.07118) | -1 | -1 |
| G: -5278.76361 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11542.53030 HOMO: -7.01782 LUMO: 0.56600 factor:1 | -1 (0.59900) | -1 | -1 |
| G: -5278.76361 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11542.71337 HOMO: -6.47359 LUMO: -0.56600 factor:1 | -1 (0.41593) | -1 | -1 |
| G: -5278.76361 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11542.40199 HOMO: -6.63686 LUMO: -0.55783 factor:1 | -1 (0.72731) | -1 | -1 |
| G: -5278.76361 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11542.93613 HOMO: -4.13885 LUMO: -2.05446 factor:1 | -1 (0.19317) | -1 | -1 |
| G: -5278.76361 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.79641 HOMO: -6.34570 LUMO: 0.19864 factor:1 | 1 (-0.66711) | -1 | -1 |
| G: -5278.76361 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.07971 HOMO: -6.47903 LUMO: 0.24762 factor:1 | 1 (-0.95041) | -1 | -1 |
| G: -5278.76361 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.56215 HOMO: -6.15249 LUMO: 0.32109 factor:1 | 1 (-0.43285) | -1 | -1 |
| G: -5278.76361 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.72787 HOMO: -6.84366 LUMO: 0.29116 factor:1 | 1 (-0.59857) | -1 | -1 |
| G: -5278.76361 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.75889 HOMO: -6.34297 LUMO: 0.19864 factor:1 | 1 (-0.62959) | -1 | -1 |
| G: -5278.76361 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.95087 HOMO: -6.51168 LUMO: 0.30749 factor:1 | 1 (-0.82157) | -1 | -1 |
| G: -5278.76361 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.48117 HOMO: -6.79468 LUMO: -0.16599 factor:1 | 1 (-0.35187) | -1 | -1 |
| G: -5278.76361 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.72477 HOMO: -7.24095 LUMO: 0.15238 factor:1 | 1 (-0.59547) | -1 | -1 |
| G: -5278.76361 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.71943 HOMO: -7.06952 LUMO: -0.34558 factor:1 | 1 (-0.59013) | -1 | -1 |
| G: -5278.76361 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.48835 HOMO: -6.88176 LUMO: 0.02177 factor:1 | 1 (-0.35905) | -1 | -1 |
| G: -5278.76361 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.46288 HOMO: -6.37291 LUMO: -0.69117 factor:1 | 1 (-0.33358) | -1 | -1 |
| G: -5278.76361 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.32979 HOMO: -6.83278 LUMO: -0.59049 factor:1 | 1 (-0.20049) | -1 | -1 |
| G: -5278.76361 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.61538 HOMO: -6.57155 LUMO: -0.33470 factor:1 | 1 (-0.48608) | -1 | -1 |
| G: -5278.76361 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.40544 HOMO: -6.89537 LUMO: -0.58504 factor:1 | 1 (-0.27614) | -1 | -1 |
| G: -5278.76361 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.49192 HOMO: -6.57155 LUMO: -0.34831 factor:1 | 1 (-0.36262) | -1 | -1 |
| G: -5278.76361 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.42316 HOMO: -6.64774 LUMO: -0.95784 factor:1 | 1 (-0.29386) | -1 | -1 |
| G: -5278.76361 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.62912 HOMO: -6.91713 LUMO: -0.69933 factor:1 | 1 (-0.49982) | -1 | -1 |
| G: -5278.76361 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.46348 HOMO: -6.80557 LUMO: -0.65035 factor:1 | 1 (-0.33418) | -1 | -1 |
| G: -5278.76361 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.34685 HOMO: -7.26544 LUMO: -0.79729 factor:1 | 1 (-0.21756) | -1 | -1 |
| G: -5278.76361 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.40473 HOMO: -6.69128 LUMO: -0.16871 factor:1 | 1 (-0.27543) | -1 | -1 |
| G: -5278.76361 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.28242 HOMO: -6.88448 LUMO: 0.13061 factor:1 | 1 (-0.15312) | -1 | -1 |
| G: -5278.76361 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.16214 HOMO: -6.50352 LUMO: 0.12245 factor:1 | 1 (-0.03284) | -1 | -1 |
| G: -5278.76361 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.59919 HOMO: -6.56067 LUMO: 0.17687 factor:1 | 1 (-0.46989) | -1 | -1 |
| G: -5278.76361 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.13441 HOMO: -6.70216 LUMO: 0.25034 factor:1 | 1 (-1.00511) | -1 | -1 |
| G: -5278.76361 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.03870 HOMO: -6.51713 LUMO: -0.78369 factor:1 | 1 (-0.90940) | -1 | -1 |
| G: -5278.76361 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.14608 HOMO: -6.50352 LUMO: 0.12245 factor:1 | 1 (-1.01678) | -1 | -1 |
| G: -5278.76361 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.88278 HOMO: -6.22052 LUMO: -0.83811 factor:1 | 1 (-0.75348) | -1 | -1 |
| G: -5278.76361 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.02668 HOMO: -6.51168 LUMO: -0.76464 factor:1 | 1 (-0.89738) | -1 | -1 |
| G: -5278.76361 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.13710 HOMO: -7.14571 LUMO: -0.80274 factor:1 | 1 (-1.00780) | -1 | -1 |
| G: -5278.76361 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.21890 HOMO: -6.66679 LUMO: -0.88709 factor:1 | 1 (-1.08960) | -1 | -1 |
| G: -5278.76361 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.83945 HOMO: -6.76203 LUMO: -1.43948 factor:1 | 1 (-1.71015) | -1 | -1 |
| G: -5278.76361 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.59534 HOMO: -6.57427 LUMO: -1.62996 factor:1 | 1 (-1.46604) | -1 | -1 |
| G: -5278.76361 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.74696 HOMO: -5.05043 LUMO: 1.24900 factor:1 | 1 (-1.61766) | -1 | -1 |
| G: -5278.76361 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.94408 HOMO: -6.53345 LUMO: 0.23130 factor:1 | 1 (-1.81478) | -1 | -1 |
| G: -5278.76361 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11545.03753 HOMO: -7.18381 LUMO: -0.22585 factor:1 | 1 (-1.90823) | -1 | -1 |
| G: -5278.76361 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11545.95278 HOMO: -7.00965 LUMO: -1.79595 factor:1 | 1 (-2.82348) | -1 | -1 |
| G: -5278.76361 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.98751 HOMO: -6.08174 LUMO: -0.82995 factor:1 | 1 (-1.85821) | -1 | -1 |
| G: -5278.76361 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.76155 HOMO: -6.42189 LUMO: -0.84355 factor:1 | 1 (-1.63225) | -1 | -1 |
| G: -5278.76361 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11545.04215 HOMO: -6.53890 LUMO: 0.60409 factor:1 | 1 (-1.91285) | -1 | -1 |
| G: -5278.76361 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11545.07467 HOMO: -6.62869 LUMO: 0.43810 factor:1 | 1 (-1.94537) | -1 | -1 |
| G: -5278.76361 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11545.11328 HOMO: -6.68312 LUMO: 0.64491 factor:1 | 1 (-1.98398) | -1 | -1 |
| G: -5278.76361 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.94269 HOMO: -6.42189 LUMO: 1.51295 factor:1 | 1 (-1.81339) | -1 | -1 |
| G: -5278.76361 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.82264 HOMO: -6.17971 LUMO: 1.67622 factor:1 | 1 (-1.69334) | -1 | -1 |
| G: -5278.76361 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.84898 HOMO: -6.79196 LUMO: 1.36873 factor:1 | 1 (-1.71968) | -1 | -1 |
| G: -5278.76361 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.78998 HOMO: -7.38517 LUMO: 0.56328 factor:1 | 1 (-1.66068) | 1 | 1 |
| G: -5278.76361 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11545.03927 HOMO: -7.56204 LUMO: 0.71566 factor:1 | 1 (-1.90997) | 1 | 1 |
| G: -5278.76361 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.63265 HOMO: -6.45726 LUMO: -1.91840 factor:1 | 1 (-1.50335) | -1 | -1 |
| G: -5278.76361 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.62954 HOMO: -6.13073 LUMO: -0.97417 factor:1 | 1 (-1.50025) | -1 | -1 |
| G: -5278.76361 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.77730 HOMO: -6.50352 LUMO: -0.69661 factor:1 | 1 (-1.64800) | -1 | -1 |
| G: -5278.76361 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.73034 HOMO: -6.76747 LUMO: -1.71976 factor:1 | 1 (-1.60104) | -1 | -1 |
| G: -5278.76361 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.61771 HOMO: -6.48447 LUMO: -0.89525 factor:1 | 1 (-1.48841) | -1 | -1 |
| G: -5278.76361 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.39659 HOMO: -7.11850 LUMO: -0.71566 factor:1 | 1 (-1.26729) | -1 | -1 |
| G: -5278.76361 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.57578 HOMO: -6.80285 LUMO: -0.49253 factor:1 | 1 (-1.44648) | -1 | -1 |
| G: -5278.76361 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.76487 HOMO: -6.80557 LUMO: -0.88165 factor:1 | 1 (-1.63557) | -1 | -1 |
| G: -5278.76361 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.85118 HOMO: -6.94162 LUMO: -0.08980 factor:1 | 1 (-1.72188) | -1 | -1 |
| G: -5278.76361 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.91818 HOMO: -6.97972 LUMO: -0.29388 factor:1 | 1 (-1.78888) | -1 | -1 |
| G: -5278.76361 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.74070 HOMO: -6.75114 LUMO: 0.04626 factor:1 | 1 (-1.61140) | -1 | -1 |
| G: -5278.76361 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.50541 HOMO: -7.15932 LUMO: 0.68845 factor:1 | 1 (-1.37611) | 1 | 1 |
| G: -5278.76361 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.71799 HOMO: -7.36612 LUMO: 0.63675 factor:1 | 1 (-0.58869) | 1 | 1 |
| G: -5278.76361 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.46299 HOMO: -7.02598 LUMO: -0.66124 factor:1 | 1 (-0.33369) | -1 | -1 |
| G: -5278.76361 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.35281 HOMO: -6.89264 LUMO: -0.54967 factor:1 | 1 (-0.22351) | -1 | -1 |
| G: -5278.76361 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.35083 HOMO: -6.97700 LUMO: 0.27756 factor:1 | 1 (-0.22153) | -1 | -1 |
| G: -5278.76361 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.22998 HOMO: -6.60965 LUMO: 0.08163 factor:1 | 1 (-0.10068) | -1 | -1 |
| G: -5278.76361 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.58207 HOMO: -6.70761 LUMO: 0.40001 factor:1 | 1 (-0.45277) | -1 | -1 |
| G: -5278.76361 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.57864 HOMO: -6.69128 LUMO: 0.23674 factor:1 | 1 (-0.44934) | -1 | -1 |
| G: -5278.76361 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.44822 HOMO: -6.69128 LUMO: -0.69933 factor:1 | 1 (-0.31892) | -1 | -1 |
| G: -5278.76361 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.85116 HOMO: -6.18515 LUMO: -0.85988 factor:1 | 1 (-0.72186) | -1 | -1 |
| G: -5278.76361 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.99323 HOMO: -6.86815 LUMO: -1.90208 factor:1 | 1 (-1.86393) | -1 | -1 |
| G: -5278.76361 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.95532 HOMO: -6.37563 LUMO: -1.74697 factor:1 | 1 (-1.82602) | -1 | -1 |
| G: -5278.76361 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.86438 HOMO: -6.75659 LUMO: 0.36463 factor:1 | 1 (-1.73508) | -1 | -1 |
| G: -5278.76361 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.75431 HOMO: -6.91441 LUMO: -0.88981 factor:1 | 1 (-1.62501) | -1 | -1 |
| G: -5278.76361 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.64392 HOMO: -6.71305 LUMO: -0.29933 factor:1 | 1 (-0.51462) | -1 | -1 |
| G: -5278.76361 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.45532 HOMO: -6.91441 LUMO: -1.04492 factor:1 | 1 (-0.32602) | -1 | -1 |
| G: -5278.76361 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.30024 HOMO: -6.05453 LUMO: -0.83539 factor:1 | 1 (-0.17094) | -1 | -1 |
| G: -5278.76361 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.37306 HOMO: -7.35252 LUMO: -0.45715 factor:1 | 1 (-0.24376) | -1 | -1 |
| G: -5278.76361 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.52773 HOMO: -6.41644 LUMO: -0.97417 factor:1 | 1 (-0.39843) | -1 | -1 |
| G: -5278.76361 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.63072 HOMO: -6.78924 LUMO: 0.36735 factor:1 | 1 (-0.50142) | -1 | -1 |
| G: -5278.76361 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11545.11769 HOMO: -6.74298 LUMO: 0.51974 factor:1 | 1 (-1.98839) | -1 | -1 |
| G: -5278.76361 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.66130 HOMO: -6.48992 LUMO: 1.44765 factor:1 | 1 (-1.53200) | -1 | -1 |
| G: -5278.76361 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.46617 HOMO: -6.12528 LUMO: 1.57826 factor:1 | 1 (-1.33687) | -1 | -1 |
| G: -5278.76361 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.25599 HOMO: -6.62325 LUMO: 1.57826 factor:1 | 1 (-1.12669) | -1 | -1 |
| G: -5278.76361 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.47885 HOMO: -6.19875 LUMO: 1.29798 factor:1 | 1 (-1.34955) | -1 | -1 |
| G: -5278.76361 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.74322 HOMO: -6.74570 LUMO: 1.52112 factor:1 | 1 (-0.61392) | -1 | -1 |
| G: -5278.76361 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.62642 HOMO: -6.84094 LUMO: 1.48574 factor:1 | 1 (-0.49712) | -1 | -1 |
| G: -5278.76361 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.69998 HOMO: -6.85183 LUMO: 0.33470 factor:1 | 1 (-0.57068) | -1 | -1 |
| G: -5278.76361 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.67214 HOMO: -6.51168 LUMO: 0.48164 factor:1 | 1 (-0.54284) | -1 | -1 |
| G: -5278.76361 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.56207 HOMO: -6.25046 LUMO: 0.75648 factor:1 | 1 (-0.43277) | -1 | -1 |
| G: -5278.76361 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.41505 HOMO: -6.65591 LUMO: 0.32109 factor:1 | 1 (-0.28575) | -1 | -1 |
| G: -5278.76361 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.37374 HOMO: -6.71033 LUMO: 0.40817 factor:1 | 1 (-0.24444) | -1 | -1 |
| G: -5278.76361 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.60019 HOMO: -6.75114 LUMO: 0.73471 factor:1 | 1 (-0.47089) | -1 | -1 |
| G: -5278.76361 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.72134 HOMO: -6.50624 LUMO: 0.59321 factor:1 | 1 (-0.59204) | -1 | -1 |
| G: -5278.76361 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.47480 HOMO: -6.39740 LUMO: 0.83267 factor:1 | 1 (-0.34550) | -1 | -1 |
| G: -5278.76361 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.52376 HOMO: -6.44094 LUMO: 0.65579 factor:1 | 1 (-0.39446) | -1 | -1 |
| G: -5278.76361 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.72047 HOMO: -6.52257 LUMO: 0.05714 factor:1 | 1 (-0.59117) | -1 | -1 |
| G: -5278.76361 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.70286 HOMO: -7.10217 LUMO: 0.49797 factor:1 | 1 (-0.57356) | -1 | -1 |
| G: -5278.76361 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.33943 HOMO: -6.83006 LUMO: 0.55783 factor:1 | 1 (-0.21013) | -1 | -1 |
| G: -5278.76361 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.49494 HOMO: -6.99333 LUMO: -0.79457 factor:1 | 1 (-0.36564) | -1 | -1 |
| G: -5278.76361 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.68917 HOMO: -6.64230 LUMO: 0.32382 factor:1 | 1 (-0.55987) | -1 | -1 |
| G: -5278.76361 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.34805 HOMO: -6.90897 LUMO: 0.30749 factor:1 | 1 (-0.21875) | -1 | -1 |
| G: -5278.76361 HOMO: -7.26544 LUMO: -1.10478 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.08846 HOMO: -7.09129 LUMO: 1.33336 factor:1 | -1 (0.04084) | 1 | 1 |
| G: -5278.76361 HOMO: -7.26544 LUMO: -1.10478 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.46552 HOMO: -6.66951 LUMO: 1.34424 factor:1 | 1 (-0.33622) | -1 | -1 |
| G: -5278.76361 HOMO: -7.26544 LUMO: -1.10478 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.51516 HOMO: -7.02870 LUMO: 1.48574 factor:1 | 1 (-0.38586) | -1 | -1 |
| G: -5278.76361 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.73903 HOMO: -7.26544 LUMO: 0.32926 factor:1 | 1 (-0.60973) | -1 | -1 |
| G: -5278.76361 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.54049 HOMO: -6.56067 LUMO: -0.45987 factor:1 | 1 (-0.41119) | -1 | -1 |
| G: -5278.76361 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.70553 HOMO: -6.54434 LUMO: -0.28300 factor:1 | 1 (-0.57623) | -1 | -1 |
| G: -5278.76361 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.70898 HOMO: -7.19469 LUMO: 0.54695 factor:1 | 1 (-0.57968) | -1 | -1 |
| G: -5278.76361 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.42492 HOMO: -6.47359 LUMO: -0.22041 factor:1 | 1 (-0.29562) | -1 | -1 |
| G: -5278.76361 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.55290 HOMO: -6.80013 LUMO: 2.08167 factor:1 | 1 (-0.42360) | -1 | -1 |
| G: -5278.76361 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.27134 HOMO: -6.23957 LUMO: 1.67894 factor:1 | 1 (-0.14204) | -1 | -1 |
| G: -5278.76361 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.62283 HOMO: -6.75114 LUMO: -0.62858 factor:1 | 1 (-0.49353) | -1 | -1 |
| G: -5278.76361 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.91070 HOMO: -6.79468 LUMO: -0.64491 factor:1 | 1 (-0.78140) | -1 | -1 |
| G: -5278.76361 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.18513 HOMO: -6.84911 LUMO: -0.69661 factor:1 | 1 (-1.05583) | -1 | -1 |
| G: -5278.76361 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.77924 HOMO: -7.54028 LUMO: 0.25851 factor:1 | 1 (-0.64994) | -1 | -1 |
| G: -5278.76361 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.72349 HOMO: -6.92802 LUMO: -0.71022 factor:1 | 1 (-0.59419) | -1 | -1 |
| G: -5278.76361 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.94899 HOMO: -6.72665 LUMO: -0.46804 factor:1 | 1 (-0.81969) | -1 | -1 |
| G: -5278.76361 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.94523 HOMO: -6.63686 LUMO: -0.23674 factor:1 | 1 (-0.81593) | -1 | -1 |
| G: -5278.76361 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.34018 HOMO: -7.21102 LUMO: 0.54423 factor:1 | 1 (-1.21088) | -1 | -1 |
| G: -5278.76361 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.53618 HOMO: -6.63414 LUMO: -0.25034 factor:1 | 1 (-1.40688) | -1 | -1 |
| G: -5278.76361 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.41915 HOMO: -6.70761 LUMO: -0.31837 factor:1 | 1 (-1.28985) | -1 | -1 |
| G: -5278.76361 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.01895 HOMO: -6.57155 LUMO: 1.76874 factor:1 | 1 (-0.88965) | -1 | -1 |
| G: -5278.76361 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.30363 HOMO: -6.84366 LUMO: 2.04358 factor:1 | 1 (-1.17433) | -1 | -1 |
| G: -5278.76361 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.25468 HOMO: -6.60420 LUMO: 1.80139 factor:1 | 1 (-1.12538) | -1 | -1 |
| G: -5278.76361 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.42130 HOMO: -7.03686 LUMO: 2.21229 factor:1 | 1 (-1.29200) | -1 | -1 |
| G: -5278.76361 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.67219 HOMO: -6.77564 LUMO: 1.97555 factor:1 | 1 (-0.54289) | -1 | -1 |
| G: -5278.76361 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.45420 HOMO: -6.40012 LUMO: 2.17691 factor:1 | 1 (-0.32490) | -1 | -1 |
| G: -5278.76361 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.54991 HOMO: -6.80013 LUMO: 2.25582 factor:1 | 1 (-0.42061) | -1 | -1 |
| G: -5278.76361 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.34645 HOMO: -6.74298 LUMO: 2.31569 factor:1 | 1 (-0.21715) | -1 | -1 |
| G: -5278.76361 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.29025 HOMO: -6.68856 LUMO: 1.85854 factor:1 | 1 (-0.16096) | -1 | -1 |
| G: -5278.76361 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.36139 HOMO: -6.17971 LUMO: 1.52928 factor:1 | 1 (-0.23209) | -1 | -1 |
| G: -5278.76361 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.52724 HOMO: -6.54162 LUMO: 1.91840 factor:1 | 1 (-0.39794) | -1 | -1 |
| G: -5278.76361 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.48675 HOMO: -6.80013 LUMO: -0.55511 factor:1 | 1 (-0.35745) | -1 | -1 |
| G: -5278.76361 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.63685 HOMO: -7.46953 LUMO: 0.28572 factor:1 | 1 (-0.50755) | -1 | -1 |
| G: -5278.76361 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.82511 HOMO: -6.61781 LUMO: -0.54967 factor:1 | 1 (-1.69581) | -1 | -1 |
| G: -5278.76361 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.60968 HOMO: -6.56339 LUMO: -0.47892 factor:1 | 1 (-1.48038) | -1 | -1 |
| G: -5278.76361 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.76462 HOMO: -6.65591 LUMO: -0.25307 factor:1 | 1 (-1.63532) | -1 | -1 |
| G: -5278.76361 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11545.60837 HOMO: -6.62869 LUMO: -0.23402 factor:1 | 1 (-2.47907) | -1 | -1 |
| G: -5278.76361 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11546.48338 HOMO: -6.58243 LUMO: -0.19048 factor:1 | 1 (-3.35408) | -1 | -1 |
| G: -5278.76361 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11546.35701 HOMO: -7.27632 LUMO: 0.52790 factor:1 | 1 (-3.22771) | -1 | -1 |
| G: -5278.76361 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11545.65909 HOMO: -7.21102 LUMO: 0.57688 factor:1 | 1 (-2.52979) | -1 | -1 |
| G: -5278.76361 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11545.48387 HOMO: -6.72393 LUMO: -0.53879 factor:1 | 1 (-2.35457) | -1 | -1 |
| G: -5278.76361 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11545.65177 HOMO: -7.42054 LUMO: -0.99322 factor:1 | 1 (-2.52247) | -1 | -1 |
| G: -5278.76361 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.90805 HOMO: -6.88992 LUMO: -0.71838 factor:1 | 1 (-1.77875) | -1 | -1 |
| G: -5278.76361 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11545.09750 HOMO: -6.88176 LUMO: -0.61226 factor:1 | 1 (-1.96820) | -1 | -1 |
| G: -5278.76361 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.67836 HOMO: -7.36340 LUMO: -1.04492 factor:1 | 1 (-1.54906) | -1 | -1 |
| G: -5278.76361 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.70765 HOMO: -6.65863 LUMO: -0.41906 factor:1 | 1 (-0.57835) | -1 | -1 |
| G: -5278.76361 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.73081 HOMO: -7.15115 LUMO: -0.66396 factor:1 | 1 (-0.60151) | -1 | -1 |
| G: -5278.76361 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.55429 HOMO: -7.10489 LUMO: -0.64491 factor:1 | 1 (-0.42499) | -1 | -1 |
| G: -5278.76361 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.49758 HOMO: -7.20285 LUMO: 0.47892 factor:1 | 1 (-0.36828) | -1 | -1 |
| G: -5278.76361 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.37513 HOMO: -6.55794 LUMO: -0.28844 factor:1 | 1 (-0.24583) | -1 | -1 |
| G: -5278.76361 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.36721 HOMO: -7.19197 LUMO: -0.69661 factor:1 | 1 (-0.23791) | -1 | -1 |
| G: -5278.76361 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.70096 HOMO: -6.56883 LUMO: -0.32926 factor:1 | 1 (-0.57166) | -1 | -1 |
| G: -5278.76361 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.55565 HOMO: -6.70761 LUMO: 1.95650 factor:1 | 1 (-0.42635) | -1 | -1 |
| G: -5278.76361 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.58838 HOMO: -6.60420 LUMO: 1.80684 factor:1 | 1 (-0.45908) | -1 | -1 |
| G: -5278.76361 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.46854 HOMO: -6.84094 LUMO: 1.64085 factor:1 | 1 (-1.33924) | -1 | -1 |
| G: -5278.76361 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.59670 HOMO: -6.69128 LUMO: 1.90208 factor:1 | 1 (-1.46740) | -1 | -1 |
| G: -5278.76361 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.58290 HOMO: -6.75387 LUMO: 1.70343 factor:1 | 1 (-1.45361) | -1 | -1 |
| G: -5278.76361 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.33289 HOMO: -7.07496 LUMO: 2.10072 factor:1 | 1 (-1.20359) | -1 | -1 |
| G: -5278.76361 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.50440 HOMO: -6.99877 LUMO: 2.24494 factor:1 | 1 (-1.37510) | -1 | -1 |
| G: -5278.76361 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.45536 HOMO: -6.63414 LUMO: 2.17691 factor:1 | 1 (-1.32607) | -1 | -1 |
| G: -5278.76361 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.42056 HOMO: -6.44638 LUMO: 1.78235 factor:1 | 1 (-1.29126) | -1 | -1 |
| G: -5278.76361 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.09933 HOMO: -6.87632 LUMO: 1.84221 factor:1 | 1 (-0.97003) | -1 | -1 |
| G: -5278.76361 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.53621 HOMO: -6.85183 LUMO: 1.68711 factor:1 | 1 (-1.40691) | -1 | -1 |
| G: -5278.76361 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.31022 HOMO: -6.96339 LUMO: 2.26671 factor:1 | 1 (-1.18092) | -1 | -1 |
| G: -5278.76361 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.96093 HOMO: -6.63141 LUMO: 1.96738 factor:1 | 1 (-0.83163) | -1 | -1 |
| G: -5278.76361 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.15974 HOMO: -6.37019 LUMO: 2.23133 factor:1 | 1 (-1.03044) | -1 | -1 |
| G: -5278.76361 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.47381 HOMO: -7.11034 LUMO: 2.32385 factor:1 | 1 (-1.34451) | 1 | 1 |
| G: -5278.76361 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.11503 HOMO: -6.91986 LUMO: 1.65445 factor:1 | 1 (-0.98573) | -1 | -1 |
| G: -5278.76361 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.38891 HOMO: -7.12938 LUMO: 2.28304 factor:1 | 1 (-1.25962) | 1 | 1 |
| G: -5278.76361 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.89148 HOMO: -6.54978 LUMO: 1.92112 factor:1 | 1 (-1.76218) | -1 | -1 |
| G: -5278.76361 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11545.11015 HOMO: -6.83006 LUMO: 2.48712 factor:1 | 1 (-1.98085) | -1 | -1 |
| G: -5278.76361 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.66359 HOMO: -6.97972 LUMO: 1.96738 factor:1 | 1 (-1.53429) | -1 | -1 |
| G: -5278.76361 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.93975 HOMO: -6.69944 LUMO: 2.06262 factor:1 | 1 (-1.81046) | -1 | -1 |
| G: -5278.76361 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.54086 HOMO: -6.76747 LUMO: 2.10888 factor:1 | 1 (-1.41156) | -1 | -1 |
| G: -5278.76361 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.78411 HOMO: -6.91169 LUMO: 2.06534 factor:1 | 1 (-1.65481) | -1 | -1 |
| G: -5278.76361 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11546.32792 HOMO: -7.03414 LUMO: 1.93473 factor:1 | 1 (-3.19862) | -1 | -1 |
| G: -5278.76361 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11545.50477 HOMO: -7.03142 LUMO: 2.52250 factor:1 | 1 (-2.37547) | -1 | -1 |
| G: -5278.76361 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11545.61841 HOMO: -6.34025 LUMO: 2.61229 factor:1 | 1 (-2.48911) | -1 | -1 |
| G: -5278.76361 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11545.56826 HOMO: -6.98788 LUMO: 2.28304 factor:1 | 1 (-2.43896) | -1 | -1 |
| G: -5278.76361 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11545.38708 HOMO: -6.97700 LUMO: 2.53882 factor:1 | 1 (-2.25778) | -1 | -1 |
| G: -5278.76361 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11545.67506 HOMO: -6.58788 LUMO: 1.94289 factor:1 | 1 (-2.54576) | -1 | -1 |
| G: -5278.76361 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.57463 HOMO: -6.78652 LUMO: 2.13609 factor:1 | 1 (-1.44533) | -1 | -1 |
| G: -5278.76361 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.68753 HOMO: -6.55250 LUMO: 1.82861 factor:1 | 1 (-1.55823) | -1 | -1 |
| G: -5278.76361 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.43874 HOMO: -6.45998 LUMO: 1.75786 factor:1 | 1 (-1.30944) | -1 | -1 |
| G: -5278.76361 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.53841 HOMO: -6.78924 LUMO: 2.33746 factor:1 | 1 (-1.40911) | -1 | -1 |
| G: -5278.76361 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.60133 HOMO: -6.85727 LUMO: 1.76058 factor:1 | 1 (-1.47203) | -1 | -1 |
| G: -5278.76361 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.76470 HOMO: -6.70489 LUMO: 1.84493 factor:1 | 1 (-1.63540) | -1 | -1 |
| G: -5278.76361 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.94662 HOMO: -6.71305 LUMO: 1.53472 factor:1 | 1 (-0.81732) | -1 | -1 |
| G: -5278.76361 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.74300 HOMO: -6.76747 LUMO: 1.48846 factor:1 | 1 (-0.61370) | -1 | -1 |
| G: -5278.76361 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.78591 HOMO: -6.69128 LUMO: 1.95922 factor:1 | 1 (-0.65661) | -1 | -1 |
| G: -5278.76361 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.70180 HOMO: -6.67495 LUMO: 2.05446 factor:1 | 1 (-0.57250) | -1 | -1 |
| G: -5278.76361 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.32514 HOMO: -6.63686 LUMO: 2.25310 factor:1 | 1 (-0.19584) | -1 | -1 |
| G: -5278.76361 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.53475 HOMO: -6.63958 LUMO: 2.14154 factor:1 | 1 (-0.40545) | -1 | -1 |
| G: -5278.76361 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.73783 HOMO: -6.62597 LUMO: 2.01908 factor:1 | 1 (-0.60853) | -1 | -1 |
| G: -5278.76361 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.35918 HOMO: -7.07768 LUMO: 2.14154 factor:1 | 1 (-0.22988) | -1 | -1 |
| G: -5278.76361 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.92420 HOMO: -6.19603 LUMO: 2.01092 factor:1 | 1 (-0.79490) | -1 | -1 |
| G: -5278.76361 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11546.09338 HOMO: -6.65046 LUMO: 2.15786 factor:1 | 1 (-2.96408) | -1 | -1 |
| G: -5278.76361 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.82158 HOMO: -6.92258 LUMO: 2.31841 factor:1 | 1 (-1.69228) | -1 | -1 |
| G: -5278.76361 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11545.71770 HOMO: -6.90081 LUMO: 2.19324 factor:1 | 1 (-2.58840) | -1 | -1 |
| G: -5278.76361 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.73575 HOMO: -6.85455 LUMO: 1.95650 factor:1 | 1 (-1.60645) | -1 | -1 |
| G: -5278.76361 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.76443 HOMO: -6.57699 LUMO: 1.76058 factor:1 | 1 (-1.63513) | -1 | -1 |
| G: -5278.76361 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.94952 HOMO: -6.90625 LUMO: 1.97555 factor:1 | 1 (-1.82022) | -1 | -1 |
| G: -5278.76361 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11545.86037 HOMO: -6.97428 LUMO: 1.92929 factor:1 | 1 (-2.73107) | -1 | -1 |
| G: -5278.76361 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.50661 HOMO: -6.61781 LUMO: -0.41906 factor:1 | 1 (-0.37731) | -1 | -1 |
| G: -5278.76361 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.68795 HOMO: -6.62869 LUMO: -0.81906 factor:1 | 1 (-0.55865) | -1 | -1 |
| G: -5278.76361 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.67761 HOMO: -7.01237 LUMO: 2.00548 factor:1 | 1 (-0.54831) | -1 | -1 |
| G: -5278.76361 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.48065 HOMO: -6.85727 LUMO: 2.17691 factor:1 | 1 (-0.35135) | -1 | -1 |
| G: -5278.76361 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.87244 HOMO: -6.71849 LUMO: 1.58914 factor:1 | 1 (-0.74314) | -1 | -1 |
| G: -5278.76361 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.99587 HOMO: -7.52395 LUMO: 0.27211 factor:1 | 1 (-0.86657) | -1 | -1 |
| G: -5278.76361 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.90346 HOMO: -6.96611 LUMO: -0.72654 factor:1 | 1 (-0.77416) | -1 | -1 |
| G: -5278.76361 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.79598 HOMO: -6.89537 LUMO: -0.68028 factor:1 | 1 (-0.66668) | -1 | -1 |
| G: -5278.76361 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.63837 HOMO: -6.84911 LUMO: -0.58504 factor:1 | 1 (-0.50907) | -1 | -1 |
| G: -5278.76361 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.51641 HOMO: -6.79196 LUMO: -0.55783 factor:1 | 1 (-0.38711) | -1 | -1 |
| G: -5278.76361 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.48405 HOMO: -6.67767 LUMO: 1.79323 factor:1 | 1 (-0.35475) | -1 | -1 |
| G: -5278.76361 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.67293 HOMO: -6.54434 LUMO: 1.91024 factor:1 | 1 (-0.54363) | -1 | -1 |
| G: -5278.76361 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11545.51664 HOMO: -6.62869 LUMO: 1.69799 factor:1 | 1 (-2.38734) | -1 | -1 |
| G: -5278.76361 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.57671 HOMO: -6.72393 LUMO: 2.12249 factor:1 | 1 (-0.44741) | -1 | -1 |
| G: -5278.76361 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.45959 HOMO: -6.66407 LUMO: 2.05990 factor:1 | 1 (-0.33029) | -1 | -1 |
| G: -5278.76361 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.49633 HOMO: -7.00149 LUMO: 1.82044 factor:1 | 1 (-0.36703) | -1 | -1 |
| G: -5278.76361 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.25031 HOMO: -7.12122 LUMO: 2.16058 factor:1 | 1 (-0.12101) | 1 | 1 |
| G: -5278.76361 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.37053 HOMO: -6.63141 LUMO: 2.21229 factor:1 | 1 (-0.24123) | -1 | -1 |
| G: -5278.76361 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.39004 HOMO: -6.37835 LUMO: 2.32113 factor:1 | 1 (-0.26074) | -1 | -1 |
| G: -5278.76361 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.16269 HOMO: -6.99605 LUMO: 2.00548 factor:1 | 1 (-0.03339) | -1 | -1 |
| G: -5278.76361 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.59959 HOMO: -6.85999 LUMO: 2.39460 factor:1 | 1 (-0.47029) | -1 | -1 |
| G: -5278.76361 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.70859 HOMO: -6.85727 LUMO: 2.48712 factor:1 | 1 (-1.57929) | -1 | -1 |
| G: -5278.76361 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.59099 HOMO: -7.04231 LUMO: 2.40277 factor:1 | 1 (-1.46169) | -1 | -1 |
| G: -5278.76361 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.64867 HOMO: -6.60692 LUMO: 2.26671 factor:1 | 1 (-1.51937) | -1 | -1 |
| G: -5278.76361 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.50889 HOMO: -6.67495 LUMO: 2.14698 factor:1 | 1 (-1.37959) | -1 | -1 |
| G: -5278.76361 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.69717 HOMO: -6.73210 LUMO: 2.06807 factor:1 | 1 (-1.56787) | -1 | -1 |
| G: -5278.76361 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11542.67261 HOMO: -7.20013 LUMO: 2.02181 factor:1 | -1 (0.45669) | 1 | 1 |
| G: -5278.76361 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11542.60771 HOMO: -7.18653 LUMO: 2.29936 factor:1 | -1 (0.52159) | 1 | 1 |
| G: -5278.76361 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11542.80521 HOMO: -6.92802 LUMO: 2.36195 factor:1 | -1 (0.32409) | -1 | -1 |
| G: -5278.76361 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.10013 HOMO: -6.89537 LUMO: 1.78779 factor:1 | -1 (0.02917) | -1 | -1 |
| G: -5278.76361 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.20832 HOMO: -6.96067 LUMO: 2.31297 factor:1 | 1 (-0.07902) | -1 | -1 |
| G: -5278.76361 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.24217 HOMO: -6.91441 LUMO: 2.50345 factor:1 | 1 (-0.11287) | -1 | -1 |
| G: -5278.76361 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.24892 HOMO: -7.17292 LUMO: 2.12521 factor:1 | 1 (-0.11962) | 1 | 1 |
| G: -5278.76361 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.56359 HOMO: -6.93618 LUMO: 2.35106 factor:1 | 1 (-0.43429) | -1 | -1 |
| G: -5278.76361 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.22903 HOMO: -6.75931 LUMO: 1.61908 factor:1 | 1 (-0.09973) | -1 | -1 |
| G: -5278.76361 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.10778 HOMO: -6.35930 LUMO: 1.23540 factor:1 | -1 (0.02152) | -1 | -1 |
| G: -5278.76361 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.46922 HOMO: -6.17971 LUMO: 1.84493 factor:1 | 1 (-0.33992) | -1 | -1 |
| G: -5278.76361 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.42057 HOMO: -6.72665 LUMO: 2.61229 factor:1 | 1 (-0.29127) | -1 | -1 |
| G: -5278.76361 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.30057 HOMO: -6.62869 LUMO: 2.28304 factor:1 | 1 (-0.17127) | -1 | -1 |
| G: -5278.76361 HOMO: -8.88180 LUMO: 1.02315 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.66210 HOMO: -6.58243 LUMO: 0.28028 factor:1 | 1 (-0.53280) | -1 | -1 |
| G: -5278.76361 HOMO: -8.88180 LUMO: 1.02315 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.51527 HOMO: -6.79468 LUMO: 0.14966 factor:1 | 1 (-0.38597) | -1 | -1 |
| G: -5278.76361 HOMO: -8.88180 LUMO: 1.02315 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.61148 HOMO: -6.63141 LUMO: 0.31021 factor:1 | 1 (-1.48218) | -1 | -1 |
| G: -5278.76361 HOMO: -8.88180 LUMO: 1.02315 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.49596 HOMO: -6.81101 LUMO: 0.13878 factor:1 | 1 (-1.36666) | -1 | -1 |
| G: -5278.76361 HOMO: -8.88180 LUMO: 1.02315 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.68993 HOMO: -6.72665 LUMO: 0.65579 factor:1 | 1 (-1.56063) | -1 | -1 |
| G: -5278.76361 HOMO: -8.88180 LUMO: 1.02315 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11542.61598 HOMO: -6.53073 LUMO: 0.91430 factor:1 | -1 (0.51332) | -1 | -1 |
| G: -5278.76361 HOMO: -8.88180 LUMO: 1.02315 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11542.43125 HOMO: -7.19197 LUMO: 1.62996 factor:1 | -1 (0.69805) | 1 | 1 |
| G: -5278.76361 HOMO: -8.88180 LUMO: 1.02315 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11542.31715 HOMO: -6.69400 LUMO: 0.84627 factor:1 | -1 (0.81215) | -1 | -1 |
| G: -5278.76361 HOMO: -8.88180 LUMO: 1.02315 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11542.50951 HOMO: -6.76475 LUMO: 0.51974 factor:1 | -1 (0.61979) | -1 | -1 |
| G: -5278.76361 HOMO: -8.88180 LUMO: 1.02315 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11542.92769 HOMO: -6.67767 LUMO: 0.52246 factor:1 | -1 (0.20161) | -1 | -1 |
| G: -5278.76361 HOMO: -8.88180 LUMO: 1.02315 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.17594 HOMO: -6.73210 LUMO: 0.94424 factor:1 | 1 (-0.04664) | -1 | -1 |
| G: -5278.76361 HOMO: -8.88180 LUMO: 1.02315 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.14130 HOMO: -6.97972 LUMO: 0.60409 factor:1 | 1 (-0.01200) | -1 | -1 |
| G: -5278.76361 HOMO: -8.88180 LUMO: 1.02315 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.02843 HOMO: -7.38517 LUMO: 0.73743 factor:1 | -1 (0.10087) | -1 | -1 |
| G: -5278.76361 HOMO: -8.88180 LUMO: 1.02315 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.22421 HOMO: -6.48992 LUMO: 1.08301 factor:1 | 1 (-0.09491) | -1 | -1 |
| G: -5278.76361 HOMO: -8.88180 LUMO: 1.02315 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.43652 HOMO: -7.18381 LUMO: 1.61908 factor:1 | 1 (-0.30722) | 1 | 1 |
| G: -5278.76361 HOMO: -8.88180 LUMO: 1.02315 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11545.92987 HOMO: -6.74842 LUMO: 0.57960 factor:1 | 1 (-2.80057) | -1 | -1 |
| G: -5278.76361 HOMO: -8.88180 LUMO: 1.02315 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.94052 HOMO: -6.67495 LUMO: 0.77280 factor:1 | 1 (-1.81122) | -1 | -1 |
| G: -5278.76361 HOMO: -8.88180 LUMO: 1.02315 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.91548 HOMO: -6.74570 LUMO: 0.77280 factor:1 | 1 (-1.78618) | -1 | -1 |
| G: -5278.76361 HOMO: -8.88180 LUMO: 1.02315 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.73877 HOMO: -6.73754 LUMO: 0.86804 factor:1 | 1 (-1.60947) | -1 | -1 |
| G: -5278.76361 HOMO: -8.88180 LUMO: 1.02315 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.94193 HOMO: -6.66135 LUMO: 0.94424 factor:1 | 1 (-1.81263) | -1 | -1 |
| G: -5278.76361 HOMO: -8.88180 LUMO: 1.02315 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.65199 HOMO: -6.44638 LUMO: 1.00138 factor:1 | 1 (-1.52269) | -1 | -1 |
| G: -5278.76361 HOMO: -8.88180 LUMO: 1.02315 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.58486 HOMO: -6.65591 LUMO: 1.02043 factor:1 | 1 (-1.45556) | -1 | -1 |
| G: -5278.76361 HOMO: -8.88180 LUMO: 1.02315 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.53069 HOMO: -7.17564 LUMO: 0.50069 factor:1 | 1 (-1.40139) | -1 | -1 |
| G: -5278.76361 HOMO: -8.88180 LUMO: 1.02315 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.40081 HOMO: -6.59332 LUMO: 0.79457 factor:1 | 1 (-1.27151) | -1 | -1 |
| G: -5278.76361 HOMO: -8.88180 LUMO: 1.02315 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.60168 HOMO: -6.76747 LUMO: 1.73881 factor:1 | 1 (-1.47238) | -1 | -1 |
| G: -5278.76361 HOMO: -8.88180 LUMO: 1.02315 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.41828 HOMO: -7.00421 LUMO: 1.07485 factor:1 | 1 (-0.28898) | -1 | -1 |
| G: -5278.76361 HOMO: -8.88180 LUMO: 1.02315 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.42329 HOMO: -6.94979 LUMO: 1.67894 factor:1 | 1 (-0.29399) | -1 | -1 |
| G: -5278.76361 HOMO: -8.88180 LUMO: 1.02315 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.24261 HOMO: -6.66135 LUMO: 0.47076 factor:1 | 1 (-0.11331) | -1 | -1 |
| G: -5278.76361 HOMO: -8.88180 LUMO: 1.02315 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.26628 HOMO: -6.74298 LUMO: 1.85037 factor:1 | 1 (-0.13698) | -1 | -1 |
| G: -5278.76361 HOMO: -8.88180 LUMO: 1.02315 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.14182 HOMO: -6.65318 LUMO: 0.95240 factor:1 | 1 (-0.01252) | -1 | -1 |
| G: -5278.76361 HOMO: -8.88180 LUMO: 1.02315 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.47336 HOMO: -6.63958 LUMO: 0.78097 factor:1 | 1 (-0.34406) | -1 | -1 |
| G: -5278.76361 HOMO: -8.88180 LUMO: 1.02315 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.33611 HOMO: -6.11712 LUMO: 0.40001 factor:1 | 1 (-0.20681) | -1 | -1 |
| G: -5278.76361 HOMO: -8.88180 LUMO: 1.02315 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.52528 HOMO: -7.08312 LUMO: 0.92519 factor:1 | 1 (-0.39598) | -1 | -1 |
| G: -5278.76361 HOMO: -8.88180 LUMO: 1.02315 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.71303 HOMO: -6.96067 LUMO: 0.54695 factor:1 | 1 (-1.58373) | -1 | -1 |
| G: -5278.76361 HOMO: -8.88180 LUMO: 1.02315 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11545.77694 HOMO: -6.74026 LUMO: 0.60137 factor:1 | 1 (-2.64764) | -1 | -1 |
| G: -5278.76361 HOMO: -8.88180 LUMO: 1.02315 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.90120 HOMO: -6.74298 LUMO: 0.59593 factor:1 | 1 (-1.77190) | -1 | -1 |
| G: -5278.76361 HOMO: -8.88180 LUMO: 1.02315 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.85352 HOMO: -6.93074 LUMO: 0.60681 factor:1 | 1 (-1.72422) | -1 | -1 |
| G: -5278.76361 HOMO: -8.88180 LUMO: 1.02315 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.88920 HOMO: -6.41644 LUMO: 0.35919 factor:1 | 1 (-1.75990) | -1 | -1 |
| G: -5278.76361 HOMO: -8.88180 LUMO: 1.02315 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.76100 HOMO: -6.41917 LUMO: 1.73064 factor:1 | 1 (-1.63170) | -1 | -1 |
| G: -5278.76361 HOMO: -8.88180 LUMO: 1.02315 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.94329 HOMO: -4.64226 LUMO: -0.87893 factor:1 | 1 (-1.81399) | -1 | -1 |
| G: -5278.76361 HOMO: -8.88180 LUMO: 1.02315 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.86781 HOMO: -6.59604 LUMO: 0.90342 factor:1 | 1 (-1.73851) | -1 | -1 |
| G: -5278.76361 HOMO: -8.88180 LUMO: 1.02315 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.50758 HOMO: -6.79468 LUMO: 0.50069 factor:1 | 1 (-1.37828) | -1 | -1 |
| G: -5278.76361 HOMO: -8.88180 LUMO: 1.02315 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.48492 HOMO: -7.04503 LUMO: 0.52518 factor:1 | 1 (-1.35562) | -1 | -1 |
| G: -5278.76361 HOMO: -8.88180 LUMO: 1.02315 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.67594 HOMO: -6.69400 LUMO: 0.54423 factor:1 | 1 (-1.54664) | -1 | -1 |
| G: -5278.76361 HOMO: -8.88180 LUMO: 1.02315 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11544.70410 HOMO: -6.51713 LUMO: 0.95240 factor:1 | 1 (-1.57480) | -1 | -1 |
| G: -5278.76361 HOMO: -8.88180 LUMO: 1.02315 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.78360 HOMO: -6.88176 LUMO: 1.79323 factor:1 | 1 (-0.65430) | -1 | -1 |
| G: -5278.76361 HOMO: -8.88180 LUMO: 1.02315 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.51875 HOMO: -6.71849 LUMO: 0.28844 factor:1 | 1 (-0.38945) | -1 | -1 |
| G: -5278.76361 HOMO: -8.88180 LUMO: 1.02315 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.70218 HOMO: -6.94979 LUMO: 0.51974 factor:1 | 1 (-0.57288) | -1 | -1 |
| G: -5278.76361 HOMO: -8.88180 LUMO: 1.02315 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.53600 HOMO: -6.76203 LUMO: 0.94151 factor:1 | 1 (-0.40670) | -1 | -1 |
| G: -5278.76361 HOMO: -8.88180 LUMO: 1.02315 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.75179 HOMO: -6.91169 LUMO: 0.89525 factor:1 | 1 (-0.62249) | -1 | -1 |
| G: -5278.76361 HOMO: -8.88180 LUMO: 1.02315 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11545.68219 HOMO: -6.83006 LUMO: 0.89253 factor:1 | 1 (-2.55289) | -1 | -1 |
| G: -5278.76361 HOMO: -8.88180 LUMO: 1.02315 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.58030 HOMO: -7.08857 LUMO: 0.60409 factor:1 | 1 (-0.45100) | -1 | -1 |
| G: -5278.76361 HOMO: -8.88180 LUMO: 1.02315 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.39782 HOMO: -6.91713 LUMO: 1.76330 factor:1 | 1 (-0.26852) | -1 | -1 |
| G: -5278.76361 HOMO: -8.88180 LUMO: 1.02315 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.50988 HOMO: -6.47359 LUMO: 1.56193 factor:1 | 1 (-0.38058) | -1 | -1 |
| G: -5278.76361 HOMO: -6.91169 LUMO: -0.53879 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.55905 HOMO: -7.00149 LUMO: 1.47214 factor:1 | 1 (-0.42975) | -1 | -1 |
| G: -5278.76361 HOMO: -6.91169 LUMO: -0.53879 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.42204 HOMO: -7.03686 LUMO: 1.97283 factor:1 | 1 (-0.29274) | -1 | -1 |
| G: -5278.76361 HOMO: -6.91169 LUMO: -0.53879 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.17197 HOMO: -7.00965 LUMO: 1.64629 factor:1 | 1 (-0.04267) | -1 | -1 |
| G: -5278.76361 HOMO: -6.91169 LUMO: -0.53879 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.61992 HOMO: -7.06952 LUMO: 1.67622 factor:1 | 1 (-0.49062) | 1 | -1 |
| G: -5278.76361 HOMO: -6.91169 LUMO: -0.53879 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.93802 HOMO: -6.80557 LUMO: 1.70615 factor:1 | 1 (-0.80872) | -1 | -1 |
| G: -5278.76361 HOMO: -6.91169 LUMO: -0.53879 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.68754 HOMO: -6.80829 LUMO: 1.71704 factor:1 | 1 (-0.55824) | -1 | -1 |
| G: -5278.76361 HOMO: -6.91169 LUMO: -0.53879 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.49178 HOMO: -7.26544 LUMO: 1.89935 factor:1 | 1 (-0.36248) | 1 | -1 |
| G: -5278.76361 HOMO: -7.29809 LUMO: 2.83543 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.25371 HOMO: -7.00149 LUMO: 1.47214 factor:1 | 1 (-0.12441) | -1 | -1 |
| G: -5278.76361 HOMO: -7.29809 LUMO: 2.83543 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.10326 HOMO: -7.03686 LUMO: 1.97283 factor:1 | -1 (0.02604) | -1 | -1 |
| G: -5278.76361 HOMO: -7.29809 LUMO: 2.83543 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.26702 HOMO: -7.00965 LUMO: 1.64629 factor:1 | 1 (-0.13772) | -1 | -1 |
| G: -5278.76361 HOMO: -7.29809 LUMO: 2.83543 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.32587 HOMO: -7.06952 LUMO: 1.67622 factor:1 | 1 (-0.19658) | -1 | -1 |
| G: -5278.76361 HOMO: -7.29809 LUMO: 2.83543 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.48087 HOMO: -6.80557 LUMO: 1.70615 factor:1 | 1 (-0.35157) | -1 | -1 |
| G: -5278.76361 HOMO: -7.29809 LUMO: 2.83543 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11543.55720 HOMO: -6.80829 LUMO: 1.71704 factor:1 | 1 (-0.42790) | -1 | -1 |
| G: -7131.05098 HOMO: -7.29809 LUMO: 2.83543 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -13396.80369 HOMO: -7.26544 LUMO: 1.89935 factor:1 | 1 (-1.38702) | -1 | -1 |
| G: -7131.05098 HOMO: -7.85865 LUMO: 2.83543 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -13394.38691 HOMO: -7.00149 LUMO: 1.75241 factor:1 | -1 (1.02976) | -1 | -1 |
| G: -7131.05098 HOMO: -7.85865 LUMO: 2.83543 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -13397.38302 HOMO: -6.91169 LUMO: 2.07079 factor:1 | 1 (-1.96635) | -1 | -1 |
| G: -7131.05098 HOMO: -7.85865 LUMO: 2.83543 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -13398.22434 HOMO: -7.11034 LUMO: 1.76330 factor:1 | 1 (-2.80767) | -1 | -1 |
| G: -7131.05098 HOMO: -7.85865 LUMO: 2.83543 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -13398.31534 HOMO: -6.87360 LUMO: 2.02725 factor:1 | 1 (-2.89867) | -1 | -1 |
| G: -7131.05098 HOMO: -7.85865 LUMO: 2.83543 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -13397.52795 HOMO: -7.08584 LUMO: 1.82044 factor:1 | 1 (-2.11128) | -1 | -1 |
| G: -7131.05098 HOMO: -7.85865 LUMO: 2.83543 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -13399.15884 HOMO: -6.90625 LUMO: 1.68166 factor:1 | 1 (-3.74216) | -1 | -1 |
| G: -7131.05098 HOMO: -7.85865 LUMO: 2.83543 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -13398.89959 HOMO: -6.71577 LUMO: 1.93201 factor:1 | 1 (-3.48292) | -1 | -1 |
| G: -7131.05098 HOMO: -7.85865 LUMO: 2.83543 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -13398.29156 HOMO: -6.99605 LUMO: 2.08439 factor:1 | 1 (-2.87488) | -1 | -1 |
| G: -7131.05098 HOMO: -7.85865 LUMO: 2.83543 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -13398.13637 HOMO: -7.02326 LUMO: 1.97010 factor:1 | 1 (-2.71970) | -1 | -1 |
| G: -7131.05098 HOMO: -7.85865 LUMO: 2.83543 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -13398.28886 HOMO: -6.99877 LUMO: 2.15514 factor:1 | 1 (-2.87219) | -1 | -1 |
| G: -7131.05098 HOMO: -7.85865 LUMO: 2.83543 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -13398.56351 HOMO: -6.75387 LUMO: 1.95106 factor:1 | 1 (-3.14683) | -1 | -1 |
| G: -7131.05098 HOMO: -7.85865 LUMO: 2.83543 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -13397.65070 HOMO: -7.10761 LUMO: 2.06262 factor:1 | 1 (-2.23403) | -1 | -1 |
| G: -7131.05098 HOMO: -7.85865 LUMO: 2.83543 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -13398.10970 HOMO: -7.03142 LUMO: 1.91568 factor:1 | 1 (-2.69303) | -1 | -1 |
| G: -7131.05098 HOMO: -7.85865 LUMO: 2.83543 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -13398.44993 HOMO: -6.98788 LUMO: 1.98371 factor:1 | 1 (-3.03325) | -1 | -1 |
| G: -7131.05098 HOMO: -7.85865 LUMO: 2.83543 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -13398.20206 HOMO: -6.94707 LUMO: 1.68438 factor:1 | 1 (-2.78538) | -1 | -1 |
| G: -7131.05098 HOMO: -7.85865 LUMO: 2.83543 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -13398.97334 HOMO: -6.88176 LUMO: 2.20684 factor:1 | 1 (-3.55666) | -1 | -1 |
| G: -7131.05098 HOMO: -7.85865 LUMO: 2.83543 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -13397.94513 HOMO: -6.73210 LUMO: 2.18780 factor:1 | 1 (-2.52845) | -1 | -1 |
| G: -7131.05098 HOMO: -7.85865 LUMO: 2.83543 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -13397.22386 HOMO: -6.83822 LUMO: 2.06807 factor:1 | 1 (-1.80719) | -1 | -1 |
| G: -7131.05098 HOMO: -7.85865 LUMO: 2.83543 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -13398.72492 HOMO: -6.78924 LUMO: 2.42181 factor:1 | 1 (-3.30825) | -1 | -1 |
| G: -7131.05098 HOMO: -7.85865 LUMO: 2.83543 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -13398.57763 HOMO: -6.94707 LUMO: 1.71704 factor:1 | 1 (-3.16096) | -1 | -1 |
| G: -7131.05098 HOMO: -7.85865 LUMO: 2.83543 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -13398.58560 HOMO: -6.85183 LUMO: 1.78779 factor:1 | 1 (-3.16893) | -1 | -1 |
| G: -7131.05098 HOMO: -7.85865 LUMO: 2.83543 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -13397.88053 HOMO: -6.98788 LUMO: 1.69799 factor:1 | 1 (-2.46385) | -1 | -1 |
| G: -7131.05098 HOMO: -7.85865 LUMO: 2.83543 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -13398.30851 HOMO: -6.79468 LUMO: 2.04358 factor:1 | 1 (-2.89184) | -1 | -1 |
| G: -7131.05098 HOMO: -7.85865 LUMO: 2.83543 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -13397.41080 HOMO: -6.90081 LUMO: 1.97283 factor:1 | 1 (-1.99413) | -1 | -1 |
| G: -7131.05098 HOMO: -7.85865 LUMO: 2.83543 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -13398.24638 HOMO: -6.79468 LUMO: 2.00820 factor:1 | 1 (-2.82971) | -1 | -1 |
| G: -7131.05098 HOMO: -7.85865 LUMO: 2.83543 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -13397.49394 HOMO: -7.06408 LUMO: 2.29936 factor:1 | 1 (-2.07726) | -1 | -1 |
| G: -7131.05098 HOMO: -7.85865 LUMO: 2.83543 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -13397.24775 HOMO: -6.78924 LUMO: 2.13337 factor:1 | 1 (-1.83108) | -1 | -1 |
| G: -7131.05098 HOMO: -7.85865 LUMO: 2.83543 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -13396.77931 HOMO: -6.79468 LUMO: 2.35106 factor:1 | 1 (-1.36264) | -1 | -1 |
| G: -7131.05098 HOMO: -7.85865 LUMO: 2.83543 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -13395.65924 HOMO: -6.82734 LUMO: 2.16603 factor:1 | 1 (-0.24256) | -1 | -1 |
| G: -7131.05098 HOMO: -7.85865 LUMO: 2.83543 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -13396.77907 HOMO: -6.79740 LUMO: 2.36739 factor:1 | 1 (-1.36239) | -1 | -1 |
| G: -7131.05098 HOMO: -7.85865 LUMO: 2.83543 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -13396.67123 HOMO: -7.14027 LUMO: 2.10888 factor:1 | 1 (-1.25455) | -1 | -1 |
| G: -7131.05098 HOMO: -6.61509 LUMO: -0.23674 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -13397.89939 HOMO: -6.96067 LUMO: 1.59731 factor:1 | 1 (-2.48271) | -1 | -1 |
| G: -7131.05098 HOMO: -6.61509 LUMO: -0.23674 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -13396.42319 HOMO: -6.91169 LUMO: 1.37145 factor:1 | 1 (-1.00652) | -1 | -1 |
| G: -7131.05098 HOMO: -6.61509 LUMO: -0.23674 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -13397.24762 HOMO: -6.94707 LUMO: 1.73064 factor:1 | 1 (-1.83095) | -1 | -1 |
| G: -7131.05098 HOMO: -6.61509 LUMO: -0.23674 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -13398.50193 HOMO: -7.02326 LUMO: 1.41227 factor:1 | 1 (-3.08525) | -1 | -1 |
| G: -7131.05098 HOMO: -6.61509 LUMO: -0.23674 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -13397.89939 HOMO: -6.72121 LUMO: 1.43132 factor:1 | 1 (-2.48271) | -1 | -1 |
| G: -7131.05098 HOMO: -6.61509 LUMO: -0.23674 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -13398.61341 HOMO: -6.51168 LUMO: 1.72520 factor:1 | 1 (-3.19674) | -1 | -1 |
| G: -7131.05098 HOMO: -6.61509 LUMO: -0.23674 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -13398.22584 HOMO: -6.98516 LUMO: 1.92929 factor:1 | 1 (-2.80917) | -1 | -1 |
| G: -7131.05098 HOMO: -6.61509 LUMO: -0.23674 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -13398.23071 HOMO: -6.92802 LUMO: 2.07895 factor:1 | 1 (-2.81404) | -1 | -1 |
| G: -7131.05098 HOMO: -6.61509 LUMO: -0.23674 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -13398.93938 HOMO: -7.02326 LUMO: 1.86398 factor:1 | 1 (-3.52270) | -1 | -1 |
| G: -7131.05098 HOMO: -6.61509 LUMO: -0.23674 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -13398.65524 HOMO: -6.82462 LUMO: 1.86670 factor:1 | 1 (-3.23856) | -1 | -1 |
| G: -7131.05098 HOMO: -6.61509 LUMO: -0.23674 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -13398.65102 HOMO: -6.83278 LUMO: 1.71160 factor:1 | 1 (-3.23435) | -1 | -1 |
| G: -7131.05098 HOMO: -6.61509 LUMO: -0.23674 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -13397.40740 HOMO: -6.62869 LUMO: 1.69527 factor:1 | 1 (-1.99073) | -1 | -1 |
| G: -7131.05098 HOMO: -6.61509 LUMO: -0.23674 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -13397.83568 HOMO: -6.84094 LUMO: 1.27349 factor:1 | 1 (-2.41901) | -1 | -1 |
| G: -7131.05098 HOMO: -6.61509 LUMO: -0.23674 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -13397.79854 HOMO: -7.07768 LUMO: 1.27621 factor:1 | 1 (-2.38187) | 1 | -1 |
| G: -7131.05098 HOMO: -6.61509 LUMO: -0.23674 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -13398.25847 HOMO: -7.06135 LUMO: 1.55105 factor:1 | 1 (-2.84179) | 1 | -1 |
| G: -7131.05098 HOMO: -6.61509 LUMO: -0.23674 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -13397.78733 HOMO: -6.94162 LUMO: 1.64629 factor:1 | 1 (-2.37066) | -1 | -1 |
| G: -7131.05098 HOMO: -6.61509 LUMO: -0.23674 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -13397.40808 HOMO: -7.07224 LUMO: 1.65445 factor:1 | 1 (-1.99141) | 1 | -1 |
| G: -7131.05098 HOMO: -6.61509 LUMO: -0.23674 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -13396.42319 HOMO: -6.68584 LUMO: 1.91296 factor:1 | 1 (-1.00652) | -1 | -1 |
| G: -7131.05098 HOMO: -6.61509 LUMO: -0.23674 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -13398.64816 HOMO: -7.09129 LUMO: 1.73609 factor:1 | 1 (-3.23149) | 1 | -1 |
| G: -7131.05098 HOMO: -6.61509 LUMO: -0.23674 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -13398.71622 HOMO: -7.01237 LUMO: 2.01092 factor:1 | 1 (-3.29954) | -1 | -1 |
| G: -7131.05098 HOMO: -6.61509 LUMO: -0.23674 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -13397.91457 HOMO: -6.93618 LUMO: 1.63540 factor:1 | 1 (-2.49790) | -1 | -1 |
| G: -7131.05098 HOMO: -6.61509 LUMO: -0.23674 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -13398.63518 HOMO: -6.98516 LUMO: 1.64629 factor:1 | 1 (-3.21851) | -1 | -1 |
| G: -7131.05098 HOMO: -6.61509 LUMO: -0.23674 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -13398.76857 HOMO: -6.80285 LUMO: 1.95106 factor:1 | 1 (-3.35190) | -1 | -1 |
| G: -7131.05098 HOMO: -6.61509 LUMO: -0.23674 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -13398.42666 HOMO: -6.76747 LUMO: 1.88303 factor:1 | 1 (-3.00999) | -1 | -1 |
| G: -7131.05098 HOMO: -6.61509 LUMO: -0.23674 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -13398.07871 HOMO: -6.64230 LUMO: 1.90480 factor:1 | 1 (-2.66204) | -1 | -1 |
| G: -7131.05098 HOMO: -6.61509 LUMO: -0.23674 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -13397.85748 HOMO: -6.93618 LUMO: 2.19324 factor:1 | 1 (-2.44081) | -1 | -1 |
| G: -7131.05098 HOMO: -6.61509 LUMO: -0.23674 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -13398.10780 HOMO: -6.95523 LUMO: 1.80684 factor:1 | 1 (-2.69112) | -1 | -1 |
| G: -7131.05098 HOMO: -6.61509 LUMO: -0.23674 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -13397.72915 HOMO: -6.66135 LUMO: 1.72792 factor:1 | 1 (-2.31248) | -1 | -1 |
| G: -7131.05098 HOMO: -6.61509 LUMO: -0.23674 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -13398.19961 HOMO: -6.36202 LUMO: 1.89391 factor:1 | 1 (-2.78294) | -1 | -1 |
| G: -7131.05098 HOMO: -6.61509 LUMO: -0.23674 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -13397.85362 HOMO: -7.03959 LUMO: 2.06262 factor:1 | 1 (-2.43694) | -1 | -1 |
| G: -7131.05098 HOMO: -6.61509 LUMO: -0.23674 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -13397.77952 HOMO: -7.08584 LUMO: 2.01092 factor:1 | 1 (-2.36285) | 1 | -1 |
| G: -7131.05098 HOMO: -6.80285 LUMO: -0.55783 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -13398.08214 HOMO: -6.96067 LUMO: 1.59731 factor:1 | 1 (-2.66546) | -1 | -1 |
| G: -7131.05098 HOMO: -6.80285 LUMO: -0.55783 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -13398.48185 HOMO: -6.91169 LUMO: 1.37145 factor:1 | 1 (-3.06517) | -1 | -1 |
| G: -7131.05098 HOMO: -6.80285 LUMO: -0.55783 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -13398.60884 HOMO: -6.94707 LUMO: 1.73064 factor:1 | 1 (-3.19217) | -1 | -1 |
| G: -7131.05098 HOMO: -6.80285 LUMO: -0.55783 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -13397.91457 HOMO: -7.02326 LUMO: 1.41227 factor:1 | 1 (-2.49790) | -1 | -1 |
| G: -7131.05098 HOMO: -6.80285 LUMO: -0.55783 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -13397.72923 HOMO: -6.72121 LUMO: 1.43132 factor:1 | 1 (-2.31256) | -1 | -1 |
| G: -7131.05098 HOMO: -6.80285 LUMO: -0.55783 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -13396.86173 HOMO: -6.51168 LUMO: 1.72520 factor:1 | 1 (-1.44506) | -1 | -1 |
| G: -7131.05098 HOMO: -6.80285 LUMO: -0.55783 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -13397.57026 HOMO: -6.98516 LUMO: 1.92929 factor:1 | 1 (-2.15359) | -1 | -1 |
| G: -7131.05098 HOMO: -6.80285 LUMO: -0.55783 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -13397.01518 HOMO: -6.92802 LUMO: 2.07895 factor:1 | 1 (-1.59851) | -1 | -1 |
| G: -7131.05098 HOMO: -6.80285 LUMO: -0.55783 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -13397.26961 HOMO: -7.02326 LUMO: 1.86398 factor:1 | 1 (-1.85293) | -1 | -1 |
| G: -7131.05098 HOMO: -6.80285 LUMO: -0.55783 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -13397.43736 HOMO: -6.82462 LUMO: 1.86670 factor:1 | 1 (-2.02069) | -1 | -1 |
| G: -7131.05098 HOMO: -6.80285 LUMO: -0.55783 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -13396.47419 HOMO: -6.83278 LUMO: 1.71160 factor:1 | 1 (-1.05752) | -1 | -1 |
| G: -7131.05098 HOMO: -6.80285 LUMO: -0.55783 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -13397.81155 HOMO: -6.62869 LUMO: 1.69527 factor:1 | 1 (-2.39487) | -1 | -1 |
| G: -7131.05098 HOMO: -6.80285 LUMO: -0.55783 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -13398.11313 HOMO: -6.84094 LUMO: 1.27349 factor:1 | 1 (-2.69646) | -1 | -1 |
| G: -7131.05098 HOMO: -6.80285 LUMO: -0.55783 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -13397.21943 HOMO: -7.07768 LUMO: 1.27621 factor:1 | 1 (-1.80275) | 1 | -1 |
| G: -7131.05098 HOMO: -6.80285 LUMO: -0.55783 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -13397.35301 HOMO: -7.06135 LUMO: 1.55105 factor:1 | 1 (-1.93634) | 1 | -1 |
| G: -7131.05098 HOMO: -6.80285 LUMO: -0.55783 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -13397.50643 HOMO: -6.94162 LUMO: 1.64629 factor:1 | 1 (-2.08975) | -1 | -1 |
| G: -7131.05098 HOMO: -6.80285 LUMO: -0.55783 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -13396.47416 HOMO: -7.07224 LUMO: 1.65445 factor:1 | 1 (-1.05749) | 1 | -1 |
| G: -7131.05098 HOMO: -6.80285 LUMO: -0.55783 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -13398.90316 HOMO: -6.68584 LUMO: 1.91296 factor:1 | 1 (-3.48649) | -1 | -1 |
| G: -7131.05098 HOMO: -6.80285 LUMO: -0.55783 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -13397.48400 HOMO: -7.09129 LUMO: 1.73609 factor:1 | 1 (-2.06733) | 1 | -1 |
| G: -7131.05098 HOMO: -6.80285 LUMO: -0.55783 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -13398.03463 HOMO: -7.01237 LUMO: 2.01092 factor:1 | 1 (-2.61795) | -1 | -1 |
| G: -7131.05098 HOMO: -6.80285 LUMO: -0.55783 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -13398.28122 HOMO: -6.93618 LUMO: 1.63540 factor:1 | 1 (-2.86454) | -1 | -1 |
| G: -7131.05098 HOMO: -6.80285 LUMO: -0.55783 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -13397.86129 HOMO: -6.98516 LUMO: 1.64629 factor:1 | 1 (-2.44462) | -1 | -1 |
| G: -7131.05098 HOMO: -6.80285 LUMO: -0.55783 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -13398.18513 HOMO: -6.80285 LUMO: 1.95106 factor:1 | 1 (-2.76846) | -1 | -1 |
| G: -7131.05098 HOMO: -6.80285 LUMO: -0.55783 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -13397.71081 HOMO: -6.76747 LUMO: 1.88303 factor:1 | 1 (-2.29414) | -1 | -1 |
| G: -7131.05098 HOMO: -6.80285 LUMO: -0.55783 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -13397.51053 HOMO: -6.64230 LUMO: 1.90480 factor:1 | 1 (-2.09386) | -1 | -1 |
| G: -7131.05098 HOMO: -6.80285 LUMO: -0.55783 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -13398.42707 HOMO: -6.93618 LUMO: 2.19324 factor:1 | 1 (-3.01040) | -1 | -1 |
| G: -7131.05098 HOMO: -6.80285 LUMO: -0.55783 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -13397.07942 HOMO: -6.95523 LUMO: 1.80684 factor:1 | 1 (-1.66275) | -1 | -1 |
| G: -7131.05098 HOMO: -6.80285 LUMO: -0.55783 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -13397.60414 HOMO: -6.66135 LUMO: 1.72792 factor:1 | 1 (-2.18747) | -1 | -1 |
| G: -7131.05098 HOMO: -6.80285 LUMO: -0.55783 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -13397.98415 HOMO: -6.36202 LUMO: 1.89391 factor:1 | 1 (-2.56748) | -1 | -1 |
| G: -7131.05098 HOMO: -6.80285 LUMO: -0.55783 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -13397.65078 HOMO: -7.03959 LUMO: 2.06262 factor:1 | 1 (-2.23411) | -1 | -1 |
| G: -7131.05098 HOMO: -6.80285 LUMO: -0.55783 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -13397.28256 HOMO: -7.08584 LUMO: 2.01092 factor:1 | 1 (-1.86588) | 1 | -1 |
| G: -7131.05098 HOMO: -7.16476 LUMO: 2.86264 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -13397.44749 HOMO: -6.96067 LUMO: 1.59731 factor:1 | 1 (-2.03081) | -1 | -1 |
| G: -7131.63148 HOMO: -7.16476 LUMO: 2.86264 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -13396.80369 HOMO: -6.91169 LUMO: 1.37145 factor:1 | 1 (-0.80652) | -1 | -1 |
| G: -7131.63148 HOMO: -7.16476 LUMO: 2.86264 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -13394.38691 HOMO: -6.94707 LUMO: 1.73064 factor:1 | -1 (1.61026) | -1 | -1 |
| G: -7131.63148 HOMO: -7.16476 LUMO: 2.86264 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -13397.38302 HOMO: -7.02326 LUMO: 1.41227 factor:1 | 1 (-1.38585) | -1 | -1 |
| G: -7131.63148 HOMO: -7.16476 LUMO: 2.86264 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -13398.22434 HOMO: -6.72121 LUMO: 1.43132 factor:1 | 1 (-2.22717) | -1 | -1 |
| G: -7131.63148 HOMO: -7.16476 LUMO: 2.86264 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -13398.31534 HOMO: -6.51168 LUMO: 1.72520 factor:1 | 1 (-2.31817) | -1 | -1 |
| G: -7131.63148 HOMO: -7.16476 LUMO: 2.86264 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -13397.52795 HOMO: -6.98516 LUMO: 1.92929 factor:1 | 1 (-1.53078) | -1 | -1 |
| G: -7131.63148 HOMO: -7.16476 LUMO: 2.86264 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -13399.15884 HOMO: -6.92802 LUMO: 2.07895 factor:1 | 1 (-3.16166) | -1 | -1 |
| G: -7131.63148 HOMO: -7.16476 LUMO: 2.86264 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -13398.89959 HOMO: -7.02326 LUMO: 1.86398 factor:1 | 1 (-2.90242) | -1 | -1 |
| G: -7131.63148 HOMO: -7.16476 LUMO: 2.86264 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -13398.29156 HOMO: -6.82462 LUMO: 1.86670 factor:1 | 1 (-2.29438) | -1 | -1 |
| G: -7131.63148 HOMO: -7.16476 LUMO: 2.86264 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -13398.13637 HOMO: -6.83278 LUMO: 1.71160 factor:1 | 1 (-2.13920) | -1 | -1 |
| G: -7131.63148 HOMO: -7.16476 LUMO: 2.86264 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -13398.28886 HOMO: -6.62869 LUMO: 1.69527 factor:1 | 1 (-2.29169) | -1 | -1 |
| G: -7131.63148 HOMO: -7.16476 LUMO: 2.86264 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -13398.56351 HOMO: -6.84094 LUMO: 1.27349 factor:1 | 1 (-2.56633) | -1 | -1 |
| G: -7131.63148 HOMO: -7.16476 LUMO: 2.86264 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -13397.65070 HOMO: -7.07768 LUMO: 1.27621 factor:1 | 1 (-1.65353) | -1 | -1 |
| G: -7131.63148 HOMO: -7.16476 LUMO: 2.86264 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -13398.10970 HOMO: -7.06135 LUMO: 1.55105 factor:1 | 1 (-2.11253) | -1 | -1 |
| G: -7131.63148 HOMO: -7.16476 LUMO: 2.86264 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -13398.44993 HOMO: -6.94162 LUMO: 1.64629 factor:1 | 1 (-2.45275) | -1 | -1 |
| G: -7131.63148 HOMO: -7.16476 LUMO: 2.86264 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -13398.20206 HOMO: -7.07224 LUMO: 1.65445 factor:1 | 1 (-2.20488) | -1 | -1 |
| G: -7131.63148 HOMO: -7.16476 LUMO: 2.86264 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -13398.97334 HOMO: -6.68584 LUMO: 1.91296 factor:1 | 1 (-2.97616) | -1 | -1 |
| G: -7131.63148 HOMO: -7.16476 LUMO: 2.86264 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -13397.94513 HOMO: -7.09129 LUMO: 1.73609 factor:1 | 1 (-1.94795) | -1 | -1 |
| G: -7131.63148 HOMO: -7.16476 LUMO: 2.86264 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -13397.22386 HOMO: -7.01237 LUMO: 2.01092 factor:1 | 1 (-1.22669) | -1 | -1 |
| G: -7131.63148 HOMO: -7.16476 LUMO: 2.86264 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -13398.72492 HOMO: -6.93618 LUMO: 1.63540 factor:1 | 1 (-2.72775) | -1 | -1 |
| G: -7131.63148 HOMO: -7.16476 LUMO: 2.86264 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -13398.57763 HOMO: -6.98516 LUMO: 1.64629 factor:1 | 1 (-2.58046) | -1 | -1 |
| G: -7131.63148 HOMO: -7.16476 LUMO: 2.86264 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -13398.58560 HOMO: -6.80285 LUMO: 1.95106 factor:1 | 1 (-2.58843) | -1 | -1 |
| G: -7131.63148 HOMO: -7.16476 LUMO: 2.86264 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -13397.88053 HOMO: -6.76747 LUMO: 1.88303 factor:1 | 1 (-1.88335) | -1 | -1 |
| G: -7131.63148 HOMO: -7.16476 LUMO: 2.86264 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -13398.30851 HOMO: -6.64230 LUMO: 1.90480 factor:1 | 1 (-2.31134) | -1 | -1 |
| G: -7131.63148 HOMO: -7.16476 LUMO: 2.86264 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -13397.41080 HOMO: -6.93618 LUMO: 2.19324 factor:1 | 1 (-1.41363) | -1 | -1 |
| G: -7131.63148 HOMO: -7.16476 LUMO: 2.86264 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -13398.24638 HOMO: -6.95523 LUMO: 1.80684 factor:1 | 1 (-2.24921) | -1 | -1 |
| G: -7131.63148 HOMO: -7.16476 LUMO: 2.86264 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -13397.49394 HOMO: -6.66135 LUMO: 1.72792 factor:1 | 1 (-1.49676) | -1 | -1 |
| G: -7131.63148 HOMO: -7.16476 LUMO: 2.86264 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -13397.24775 HOMO: -6.36202 LUMO: 1.89391 factor:1 | 1 (-1.25058) | -1 | -1 |
| G: -7131.63148 HOMO: -7.16476 LUMO: 2.86264 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -13396.77931 HOMO: -7.03959 LUMO: 2.06262 factor:1 | 1 (-0.78214) | -1 | -1 |
| G: -7131.63148 HOMO: -7.16476 LUMO: 2.86264 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -13395.65924 HOMO: -7.08584 LUMO: 2.01092 factor:1 | -1 (0.33794) | -1 | -1 |
| G: -7131.63148 HOMO: -6.50352 LUMO: 2.10888 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -13396.77907 HOMO: -6.96067 LUMO: 1.59731 factor:1 | 1 (-0.78189) | 1 | 1 |
| G: -7131.63148 HOMO: -6.50352 LUMO: 2.10888 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -13396.67123 HOMO: -6.91169 LUMO: 1.37145 factor:1 | 1 (-0.67405) | -1 | -1 |
| G: -7131.63148 HOMO: -6.50352 LUMO: 2.10888 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -13397.89939 HOMO: -6.94707 LUMO: 1.73064 factor:1 | 1 (-1.90221) | 1 | 1 |
| G: -7131.63148 HOMO: -6.50352 LUMO: 2.10888 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -13396.42319 HOMO: -7.02326 LUMO: 1.41227 factor:1 | 1 (-0.42602) | -1 | -1 |
| G: -7131.63148 HOMO: -6.50352 LUMO: 2.10888 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -13397.24762 HOMO: -6.72121 LUMO: 1.43132 factor:1 | 1 (-1.25044) | -1 | -1 |
| G: -7131.63148 HOMO: -6.50352 LUMO: 2.10888 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -13398.50193 HOMO: -6.51168 LUMO: 1.72520 factor:1 | 1 (-2.50475) | 1 | 1 |
| G: -7131.63148 HOMO: -6.50352 LUMO: 2.10888 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -13397.89939 HOMO: -6.98516 LUMO: 1.92929 factor:1 | 1 (-1.90221) | 1 | 1 |
| G: -7131.63148 HOMO: -6.50352 LUMO: 2.10888 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -13398.61341 HOMO: -6.92802 LUMO: 2.07895 factor:1 | 1 (-2.61624) | 1 | 1 |
| G: -7131.63148 HOMO: -6.50352 LUMO: 2.10888 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -13398.22584 HOMO: -7.02326 LUMO: 1.86398 factor:1 | 1 (-2.22867) | 1 | 1 |
| G: -7131.63148 HOMO: -6.50352 LUMO: 2.10888 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -13398.23071 HOMO: -6.82462 LUMO: 1.86670 factor:1 | 1 (-2.23354) | 1 | 1 |
| G: -7131.63148 HOMO: -6.50352 LUMO: 2.10888 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -13398.93938 HOMO: -6.83278 LUMO: 1.71160 factor:1 | 1 (-2.94220) | 1 | 1 |
| G: -7131.63148 HOMO: -6.50352 LUMO: 2.10888 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -13398.65524 HOMO: -6.62869 LUMO: 1.69527 factor:1 | 1 (-2.65806) | 1 | 1 |
| G: -7131.63148 HOMO: -6.50352 LUMO: 2.10888 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -13398.65102 HOMO: -6.84094 LUMO: 1.27349 factor:1 | 1 (-2.65384) | -1 | -1 |
| G: -7131.63148 HOMO: -6.50352 LUMO: 2.10888 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -13397.40740 HOMO: -7.07768 LUMO: 1.27621 factor:1 | 1 (-1.41023) | -1 | -1 |
| G: -7131.63148 HOMO: -6.50352 LUMO: 2.10888 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -13397.83568 HOMO: -7.06135 LUMO: 1.55105 factor:1 | 1 (-1.83851) | -1 | -1 |
| G: -7131.63148 HOMO: -6.50352 LUMO: 2.10888 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -13397.79854 HOMO: -6.94162 LUMO: 1.64629 factor:1 | 1 (-1.80137) | 1 | 1 |
| G: -7131.63148 HOMO: -6.50352 LUMO: 2.10888 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -13398.25847 HOMO: -7.07224 LUMO: 1.65445 factor:1 | 1 (-2.26129) | 1 | 1 |
| G: -7131.63148 HOMO: -6.50352 LUMO: 2.10888 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -13397.78733 HOMO: -6.68584 LUMO: 1.91296 factor:1 | 1 (-1.79016) | 1 | 1 |
| G: -7131.63148 HOMO: -6.50352 LUMO: 2.10888 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -13397.40808 HOMO: -7.09129 LUMO: 1.73609 factor:1 | 1 (-1.41091) | 1 | 1 |
| G: -7131.63148 HOMO: -6.50352 LUMO: 2.10888 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -13396.42319 HOMO: -7.01237 LUMO: 2.01092 factor:1 | 1 (-0.42602) | 1 | 1 |
| G: -7131.63148 HOMO: -6.50352 LUMO: 2.10888 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -13398.64816 HOMO: -6.93618 LUMO: 1.63540 factor:1 | 1 (-2.65099) | 1 | 1 |
| G: -7131.63148 HOMO: -6.50352 LUMO: 2.10888 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -13398.71622 HOMO: -6.98516 LUMO: 1.64629 factor:1 | 1 (-2.71904) | 1 | 1 |
| G: -7131.63148 HOMO: -6.50352 LUMO: 2.10888 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -13397.91457 HOMO: -6.80285 LUMO: 1.95106 factor:1 | 1 (-1.91740) | 1 | 1 |
| G: -7131.63148 HOMO: -6.50352 LUMO: 2.10888 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -13398.63518 HOMO: -6.76747 LUMO: 1.88303 factor:1 | 1 (-2.63801) | 1 | 1 |
| G: -7131.63148 HOMO: -6.50352 LUMO: 2.10888 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -13398.76857 HOMO: -6.64230 LUMO: 1.90480 factor:1 | 1 (-2.77140) | 1 | 1 |
| G: -7131.63148 HOMO: -6.50352 LUMO: 2.10888 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -13398.42666 HOMO: -6.93618 LUMO: 2.19324 factor:1 | 1 (-2.42949) | 1 | 1 |
| G: -7131.63148 HOMO: -6.50352 LUMO: 2.10888 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -13398.07871 HOMO: -6.95523 LUMO: 1.80684 factor:1 | 1 (-2.08153) | 1 | 1 |
| G: -7131.63148 HOMO: -6.50352 LUMO: 2.10888 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -13397.85748 HOMO: -6.66135 LUMO: 1.72792 factor:1 | 1 (-1.86031) | 1 | 1 |
| G: -7131.63148 HOMO: -6.50352 LUMO: 2.10888 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -13398.10780 HOMO: -6.36202 LUMO: 1.89391 factor:1 | 1 (-2.11062) | -1 | -1 |
| G: -7131.63148 HOMO: -6.50352 LUMO: 2.10888 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -13397.72915 HOMO: -7.03959 LUMO: 2.06262 factor:1 | 1 (-1.73198) | 1 | 1 |
| G: -7131.63148 HOMO: -6.50352 LUMO: 2.10888 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -13398.19961 HOMO: -7.08584 LUMO: 2.01092 factor:1 | 1 (-2.20244) | 1 | 1 |
| G: -7131.63148 HOMO: -6.59604 LUMO: 2.33746 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -13397.85362 HOMO: -6.96067 LUMO: 1.59731 factor:1 | 1 (-1.85644) | 1 | 1 |
| G: -7131.63148 HOMO: -6.59604 LUMO: 2.33746 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -13397.77952 HOMO: -6.91169 LUMO: 1.37145 factor:1 | 1 (-1.78235) | -1 | -1 |
| G: -7131.63148 HOMO: -6.59604 LUMO: 2.33746 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -13398.08214 HOMO: -6.94707 LUMO: 1.73064 factor:1 | 1 (-2.08496) | 1 | 1 |
| G: -7131.63148 HOMO: -6.59604 LUMO: 2.33746 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -13398.48185 HOMO: -7.02326 LUMO: 1.41227 factor:1 | 1 (-2.48467) | -1 | -1 |
| G: -7131.63148 HOMO: -6.59604 LUMO: 2.33746 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -13398.60884 HOMO: -6.72121 LUMO: 1.43132 factor:1 | 1 (-2.61167) | -1 | -1 |
| G: -7131.63148 HOMO: -6.59604 LUMO: 2.33746 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -13397.91457 HOMO: -6.51168 LUMO: 1.72520 factor:1 | 1 (-1.91740) | -1 | -1 |
| G: -7131.63148 HOMO: -6.59604 LUMO: 2.33746 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -13397.72923 HOMO: -6.98516 LUMO: 1.92929 factor:1 | 1 (-1.73206) | 1 | 1 |
| G: -7131.63148 HOMO: -6.59604 LUMO: 2.33746 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -13396.86173 HOMO: -6.92802 LUMO: 2.07895 factor:1 | 1 (-0.86456) | 1 | 1 |
| G: -7131.63148 HOMO: -6.59604 LUMO: 2.33746 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -13397.57026 HOMO: -7.02326 LUMO: 1.86398 factor:1 | 1 (-1.57309) | 1 | 1 |
| G: -7131.63148 HOMO: -6.59604 LUMO: 2.33746 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -13397.01518 HOMO: -6.82462 LUMO: 1.86670 factor:1 | 1 (-1.01801) | 1 | 1 |
| G: -7131.63148 HOMO: -6.59604 LUMO: 2.33746 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -13397.26961 HOMO: -6.83278 LUMO: 1.71160 factor:1 | 1 (-1.27243) | 1 | 1 |
| G: -7131.63148 HOMO: -6.59604 LUMO: 2.33746 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -13397.43736 HOMO: -6.62869 LUMO: 1.69527 factor:1 | 1 (-1.44019) | 1 | 1 |
| G: -7131.63148 HOMO: -6.59604 LUMO: 2.33746 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -13396.47419 HOMO: -6.84094 LUMO: 1.27349 factor:1 | 1 (-0.47702) | -1 | -1 |
| G: -7131.63148 HOMO: -6.59604 LUMO: 2.33746 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -13397.81155 HOMO: -7.07768 LUMO: 1.27621 factor:1 | 1 (-1.81437) | -1 | -1 |
| G: -7131.63148 HOMO: -6.59604 LUMO: 2.33746 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -13398.11313 HOMO: -7.06135 LUMO: 1.55105 factor:1 | 1 (-2.11596) | -1 | -1 |
| G: -7131.63148 HOMO: -6.59604 LUMO: 2.33746 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -13397.21943 HOMO: -6.94162 LUMO: 1.64629 factor:1 | 1 (-1.22225) | 1 | 1 |
| G: -7131.63148 HOMO: -6.59604 LUMO: 2.33746 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -13397.35301 HOMO: -7.07224 LUMO: 1.65445 factor:1 | 1 (-1.35583) | 1 | 1 |
| G: -7131.63148 HOMO: -6.59604 LUMO: 2.33746 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -13397.50643 HOMO: -6.68584 LUMO: 1.91296 factor:1 | 1 (-1.50925) | 1 | 1 |
| G: -7131.63148 HOMO: -6.59604 LUMO: 2.33746 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -13396.47416 HOMO: -7.09129 LUMO: 1.73609 factor:1 | 1 (-0.47699) | 1 | 1 |
| G: -7131.63148 HOMO: -6.59604 LUMO: 2.33746 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -13398.90316 HOMO: -7.01237 LUMO: 2.01092 factor:1 | 1 (-2.90599) | 1 | 1 |
| G: -7131.63148 HOMO: -6.59604 LUMO: 2.33746 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -13397.48400 HOMO: -6.93618 LUMO: 1.63540 factor:1 | 1 (-1.48683) | 1 | 1 |
| G: -7131.63148 HOMO: -6.59604 LUMO: 2.33746 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -13398.03463 HOMO: -6.98516 LUMO: 1.64629 factor:1 | 1 (-2.03745) | 1 | 1 |
| G: -7131.63148 HOMO: -6.59604 LUMO: 2.33746 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -13398.28122 HOMO: -6.80285 LUMO: 1.95106 factor:1 | 1 (-2.28404) | 1 | 1 |
| G: -7131.63148 HOMO: -6.59604 LUMO: 2.33746 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -13397.86129 HOMO: -6.76747 LUMO: 1.88303 factor:1 | 1 (-1.86412) | 1 | 1 |
| G: -7131.63148 HOMO: -6.59604 LUMO: 2.33746 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -13398.18513 HOMO: -6.64230 LUMO: 1.90480 factor:1 | 1 (-2.18796) | 1 | 1 |
| G: -7131.63148 HOMO: -6.59604 LUMO: 2.33746 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -13397.71081 HOMO: -6.93618 LUMO: 2.19324 factor:1 | 1 (-1.71364) | 1 | 1 |
| G: -7131.63148 HOMO: -6.59604 LUMO: 2.33746 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -13397.51053 HOMO: -6.95523 LUMO: 1.80684 factor:1 | 1 (-1.51336) | 1 | 1 |
| G: -7131.63148 HOMO: -6.59604 LUMO: 2.33746 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -13398.42707 HOMO: -6.66135 LUMO: 1.72792 factor:1 | 1 (-2.42990) | 1 | 1 |
| G: -7131.63148 HOMO: -6.59604 LUMO: 2.33746 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -13397.07942 HOMO: -6.36202 LUMO: 1.89391 factor:1 | 1 (-1.08225) | -1 | -1 |
| G: -7131.63148 HOMO: -6.59604 LUMO: 2.33746 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -13397.60414 HOMO: -7.03959 LUMO: 2.06262 factor:1 | 1 (-1.60697) | 1 | 1 |
| G: -7131.63148 HOMO: -6.59604 LUMO: 2.33746 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -13397.98415 HOMO: -7.08584 LUMO: 2.01092 factor:1 | 1 (-1.98698) | 1 | 1 |
| G: -7131.63148 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -13397.65078 HOMO: -7.06135 LUMO: 0.75376 factor:1 | 1 (-1.65361) | 1 | -1 |
| G: -7131.63148 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -13397.28256 HOMO: -5.10213 LUMO: 0.77825 factor:1 | 1 (-1.28538) | -1 | -1 |
| G: -7131.63148 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -13397.44749 HOMO: -5.84228 LUMO: 0.50341 factor:1 | 1 (-1.45031) | -1 | -1 |
| G: -7131.87521 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -13396.80369 HOMO: -5.39874 LUMO: 0.68028 factor:1 | 1 (-0.56279) | -1 | -1 |
| G: -7131.87521 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -13394.38691 HOMO: -5.16744 LUMO: 1.14832 factor:1 | -1 (1.85399) | -1 | -1 |
| G: -7131.87521 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -13397.38302 HOMO: -5.80963 LUMO: 0.35647 factor:1 | 1 (-1.14212) | -1 | -1 |
| G: -7131.87521 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -13398.22434 HOMO: -5.02322 LUMO: 1.07213 factor:1 | 1 (-1.98344) | -1 | -1 |
| G: -7131.87521 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -13398.31534 HOMO: -5.80963 LUMO: 0.56328 factor:1 | 1 (-2.07443) | -1 | -1 |
| G: -7131.87521 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -13397.52795 HOMO: -5.45316 LUMO: 0.78369 factor:1 | 1 (-1.28704) | -1 | -1 |
| G: -7131.87521 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -13399.15884 HOMO: -5.25452 LUMO: 0.82178 factor:1 | 1 (-2.91793) | -1 | -1 |
| G: -7131.87521 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -13398.89959 HOMO: -5.21370 LUMO: 1.03947 factor:1 | 1 (-2.65869) | -1 | -1 |
| G: -7131.87521 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -13398.29156 HOMO: -6.04365 LUMO: 0.31837 factor:1 | 1 (-2.05065) | -1 | -1 |
| G: -7131.87521 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -13398.13637 HOMO: -5.86405 LUMO: 0.55511 factor:1 | 1 (-1.89546) | -1 | -1 |
| G: -7131.87521 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -13398.28886 HOMO: -5.64908 LUMO: 0.71022 factor:1 | 1 (-2.04796) | -1 | -1 |
| G: -7131.87521 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -13398.56351 HOMO: -5.94297 LUMO: 0.68301 factor:1 | 1 (-2.32260) | -1 | -1 |
| G: -7131.87521 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -13397.65070 HOMO: -6.01916 LUMO: 0.56328 factor:1 | 1 (-1.40979) | -1 | -1 |
| G: -7131.87521 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -13398.10970 HOMO: -6.05181 LUMO: 0.35103 factor:1 | 1 (-1.86880) | -1 | -1 |
| G: -7131.87521 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -13398.44993 HOMO: -6.08447 LUMO: 0.48436 factor:1 | 1 (-2.20902) | -1 | -1 |
| G: -7131.87521 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -13398.20206 HOMO: -5.86950 LUMO: 0.36735 factor:1 | 1 (-1.96115) | -1 | -1 |
| G: -7131.87521 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -13398.97334 HOMO: -5.33615 LUMO: 0.65852 factor:1 | 1 (-2.73243) | -1 | -1 |
| G: -7131.87521 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -13397.94513 HOMO: -5.36064 LUMO: 0.86804 factor:1 | 1 (-1.70422) | -1 | -1 |
| G: -7131.87521 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -13397.22386 HOMO: -5.74160 LUMO: 0.64491 factor:1 | 1 (-0.98296) | -1 | -1 |
| G: -7131.87521 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -13398.72492 HOMO: -5.23003 LUMO: 0.66124 factor:1 | 1 (-2.48402) | -1 | -1 |
| G: -7131.87521 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -13398.57763 HOMO: -5.77698 LUMO: 0.84083 factor:1 | 1 (-2.33672) | -1 | -1 |
| G: -7131.87521 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -13398.58560 HOMO: -5.60555 LUMO: 0.84355 factor:1 | 1 (-2.34470) | -1 | -1 |
| G: -7131.87521 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -13397.88053 HOMO: -7.11578 LUMO: -1.62452 factor:1 | 1 (-1.63962) | -1 | -1 |
| G: -7131.87521 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -13398.30851 HOMO: -7.23279 LUMO: -1.63813 factor:1 | 1 (-2.06760) | -1 | -1 |
| G: -7131.87521 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -13397.41080 HOMO: -6.68312 LUMO: -0.88709 factor:1 | 1 (-1.16990) | -1 | -1 |
| G: -7131.87521 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -13398.24638 HOMO: -6.99333 LUMO: -0.88709 factor:1 | 1 (-2.00548) | -1 | -1 |
| G: -7131.87521 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -13397.49394 HOMO: -7.40694 LUMO: 0.11973 factor:1 | 1 (-1.25303) | 1 | 1 |
| G: -7131.87521 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -13397.24775 HOMO: -6.74026 LUMO: -0.72927 factor:1 | 1 (-1.00685) | -1 | -1 |
| G: -7131.87521 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -13396.77931 HOMO: -6.67223 LUMO: -0.70750 factor:1 | 1 (-0.53840) | -1 | -1 |
| G: -7131.87521 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -13395.65924 HOMO: -7.06952 LUMO: -1.40139 factor:1 | -1 (0.58167) | -1 | -1 |
| G: -7131.87521 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -13396.77907 HOMO: -7.21374 LUMO: -1.13199 factor:1 | 1 (-0.53816) | -1 | -1 |
| G: -7131.87521 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -13396.67123 HOMO: -6.54706 LUMO: -1.34424 factor:1 | 1 (-0.43032) | -1 | -1 |
| G: -7131.87521 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -13397.89939 HOMO: -7.51851 LUMO: -1.05852 factor:1 | 1 (-1.65848) | -1 | -1 |
| G: -7131.87521 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -13396.42319 HOMO: -7.07224 LUMO: -1.89391 factor:1 | 1 (-0.18229) | -1 | -1 |
| G: -7131.87521 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -13397.24762 HOMO: -6.65863 LUMO: -0.46804 factor:1 | 1 (-1.00671) | -1 | -1 |
| G: -7131.87521 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -13398.50193 HOMO: -7.24367 LUMO: 0.29388 factor:1 | 1 (-2.26102) | 1 | 1 |
| G: -7131.87521 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -13397.89939 HOMO: -7.02326 LUMO: -0.87893 factor:1 | 1 (-1.65848) | -1 | -1 |
| G: -7131.87521 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -13398.61341 HOMO: -6.88176 LUMO: 0.71566 factor:1 | 1 (-2.37251) | -1 | -1 |
| G: -7131.87521 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -13398.22584 HOMO: -6.46543 LUMO: 1.01498 factor:1 | 1 (-1.98493) | -1 | -1 |
| G: -7131.87521 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -13398.23071 HOMO: -6.30760 LUMO: 0.17687 factor:1 | 1 (-1.98981) | -1 | -1 |
| G: -7131.87521 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -13398.93938 HOMO: -6.73210 LUMO: -1.06941 factor:1 | 1 (-2.69847) | -1 | -1 |
| G: -7131.87521 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -13398.65524 HOMO: -6.83550 LUMO: -0.75920 factor:1 | 1 (-2.41433) | -1 | -1 |
| G: -7131.87521 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -13398.65102 HOMO: -6.94707 LUMO: 0.42178 factor:1 | 1 (-2.41011) | -1 | -1 |
| G: -7131.87521 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -13397.40740 HOMO: -6.77019 LUMO: -0.38096 factor:1 | 1 (-1.16650) | -1 | -1 |
| G: -7131.87521 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -13397.83568 HOMO: -7.34163 LUMO: 0.35103 factor:1 | 1 (-1.59478) | 1 | 1 |
| G: -7131.87521 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -13397.79854 HOMO: -6.87632 LUMO: -0.87349 factor:1 | 1 (-1.55763) | -1 | -1 |
| G: -7131.87521 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -13398.25847 HOMO: -7.06952 LUMO: -1.47214 factor:1 | 1 (-2.01756) | -1 | -1 |
| G: -7131.87521 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -13397.78733 HOMO: -6.58788 LUMO: -0.37824 factor:1 | 1 (-1.54642) | -1 | -1 |
| G: -7131.87521 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -13397.40808 HOMO: -6.92802 LUMO: -1.24900 factor:1 | 1 (-1.16718) | -1 | -1 |
| G: -7131.87521 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -13396.42319 HOMO: -7.01237 LUMO: -1.31975 factor:1 | 1 (-0.18229) | -1 | -1 |
| G: -7131.87521 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -13398.64816 HOMO: -6.74842 LUMO: 0.45987 factor:1 | 1 (-2.40726) | -1 | -1 |
| G: -7131.87521 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -13398.71622 HOMO: -6.53890 LUMO: 0.94424 factor:1 | 1 (-2.47531) | -1 | -1 |
| G: -7131.87521 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -13397.91457 HOMO: -6.52257 LUMO: -0.66940 factor:1 | 1 (-1.67366) | -1 | -1 |
| G: -7131.87521 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -13398.63518 HOMO: -6.56883 LUMO: -1.48302 factor:1 | 1 (-2.39428) | -1 | -1 |
| G: -7131.87521 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -13398.76857 HOMO: -7.21646 LUMO: 0.13061 factor:1 | 1 (-2.52767) | 1 | 1 |
| G: -7131.87521 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -13398.42666 HOMO: -6.62597 LUMO: -0.64763 factor:1 | 1 (-2.18575) | -1 | -1 |
| G: -7131.87521 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -13398.07871 HOMO: -7.38789 LUMO: 0.31021 factor:1 | 1 (-1.83780) | 1 | 1 |
| G: -7131.87521 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -13397.85748 HOMO: -6.74570 LUMO: -0.70750 factor:1 | 1 (-1.61657) | -1 | -1 |
| G: -7131.87521 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -13398.10780 HOMO: -6.95251 LUMO: -1.25989 factor:1 | 1 (-1.86689) | -1 | -1 |
| G: -7131.87521 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -13397.72915 HOMO: -7.13483 LUMO: -0.76736 factor:1 | 1 (-1.48825) | -1 | -1 |
| G: -7131.87521 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -13398.19961 HOMO: -6.93618 LUMO: -1.24628 factor:1 | 1 (-1.95870) | -1 | -1 |
| G: -7131.87521 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -13397.85362 HOMO: -7.03686 LUMO: 0.26395 factor:1 | 1 (-1.61271) | -1 | -1 |
| G: -7131.87521 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -13397.77952 HOMO: -6.52257 LUMO: -0.84355 factor:1 | 1 (-1.53861) | -1 | -1 |
| G: -7131.87521 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -13398.08214 HOMO: -6.83278 LUMO: -0.49525 factor:1 | 1 (-1.84123) | -1 | -1 |
| G: -7131.87521 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -13398.48185 HOMO: -7.18381 LUMO: -1.64629 factor:1 | 1 (-2.24094) | -1 | -1 |
| G: -7131.87521 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -13398.60884 HOMO: -6.74842 LUMO: -0.81090 factor:1 | 1 (-2.36793) | -1 | -1 |
| G: -7131.87521 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -13397.91457 HOMO: -7.09401 LUMO: -0.92519 factor:1 | 1 (-1.67366) | -1 | -1 |
| G: -7131.87521 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -13397.72923 HOMO: -7.20285 LUMO: -0.81634 factor:1 | 1 (-1.48833) | -1 | -1 |
| G: -7131.87521 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -13396.86173 HOMO: -6.72665 LUMO: 0.77008 factor:1 | 1 (-0.62083) | -1 | -1 |
| G: -7131.87521 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -13397.57026 HOMO: -6.80829 LUMO: 0.86532 factor:1 | 1 (-1.32936) | -1 | -1 |
| G: -7131.87521 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -13397.01518 HOMO: -6.20964 LUMO: 0.99866 factor:1 | 1 (-0.77427) | -1 | -1 |
| G: -7131.87521 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -13397.26961 HOMO: -6.52801 LUMO: 1.07757 factor:1 | 1 (-1.02870) | -1 | -1 |
| G: -7131.87521 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -13397.43736 HOMO: -6.74298 LUMO: -0.67756 factor:1 | 1 (-1.19646) | -1 | -1 |
| G: -7131.87521 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -13396.47419 HOMO: -7.43959 LUMO: 0.03265 factor:1 | 1 (-0.23328) | 1 | 1 |
| G: -7131.87521 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -13397.81155 HOMO: -6.46815 LUMO: -0.29933 factor:1 | 1 (-1.57064) | -1 | -1 |
| G: -7131.87521 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -13398.11313 HOMO: -6.70489 LUMO: -0.97145 factor:1 | 1 (-1.87222) | -1 | -1 |
| G: -7131.87521 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -13397.21943 HOMO: -6.30216 LUMO: -1.39322 factor:1 | 1 (-0.97852) | -1 | -1 |
| G: -7131.87521 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -13397.35301 HOMO: -7.01782 LUMO: -1.07485 factor:1 | 1 (-1.11210) | -1 | -1 |
| G: -7131.87521 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -13397.50643 HOMO: -6.93074 LUMO: 0.25851 factor:1 | 1 (-1.26552) | -1 | -1 |
| G: -7131.87521 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -13396.47416 HOMO: -7.07224 LUMO: 0.09524 factor:1 | 1 (-0.23326) | 1 | 1 |
| G: -7131.87521 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -13398.90316 HOMO: -6.62325 LUMO: -0.45443 factor:1 | 1 (-2.66225) | -1 | -1 |
| G: -7131.87521 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -13397.48400 HOMO: -7.09945 LUMO: -1.20274 factor:1 | 1 (-1.24310) | -1 | -1 |
| G: -7131.87521 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -13398.03463 HOMO: -6.56067 LUMO: -1.39322 factor:1 | 1 (-1.79372) | -1 | -1 |
| G: -7131.87521 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -13398.28122 HOMO: -6.75387 LUMO: -0.72654 factor:1 | 1 (-2.04031) | -1 | -1 |
| G: -7131.87521 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -13397.86129 HOMO: -6.28583 LUMO: -2.35651 factor:1 | 1 (-1.62038) | -1 | -1 |
| G: -7131.87521 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -13398.18513 HOMO: -6.55522 LUMO: -1.33608 factor:1 | 1 (-1.94423) | -1 | -1 |
| G: -7131.87521 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -13397.71081 HOMO: -7.19741 LUMO: -0.93607 factor:1 | 1 (-1.46990) | -1 | -1 |
| G: -7131.87521 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -13397.51053 HOMO: -6.39740 LUMO: -1.14832 factor:1 | 1 (-1.26963) | -1 | -1 |
| G: -7131.87521 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -13398.42707 HOMO: -7.11850 LUMO: -0.97417 factor:1 | 1 (-2.18616) | -1 | -1 |
| G: -7131.87521 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -13397.07942 HOMO: -6.57699 LUMO: -1.14016 factor:1 | 1 (-0.83852) | -1 | -1 |
| G: -7131.87521 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -13397.60414 HOMO: -6.57699 LUMO: -1.31975 factor:1 | 1 (-1.36324) | -1 | -1 |
| G: -7131.87521 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -13397.98415 HOMO: -6.69128 LUMO: -0.76736 factor:1 | 1 (-1.74324) | -1 | -1 |
| G: -7131.87521 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -13397.65078 HOMO: -7.25728 LUMO: 0.29660 factor:1 | 1 (-1.40988) | 1 | 1 |
| G: -7131.87521 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -13397.28256 HOMO: -6.37019 LUMO: -0.95240 factor:1 | 1 (-1.04165) | -1 | -1 |
| G: -7131.87521 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -13397.44749 HOMO: -6.48447 LUMO: -0.55511 factor:1 | 1 (-1.20658) | -1 | -1 |
| G: -7130.57649 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -13396.80369 HOMO: -6.37291 LUMO: -0.78641 factor:1 | 1 (-1.86150) | -1 | -1 |
| G: -7130.57649 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -13394.38691 HOMO: -6.65863 LUMO: -0.69933 factor:1 | -1 (0.55528) | -1 | -1 |
| G: -7130.57649 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -13397.38302 HOMO: -6.44638 LUMO: -0.16055 factor:1 | 1 (-2.44083) | -1 | -1 |
| G: -7130.57649 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -13398.22434 HOMO: -6.41917 LUMO: -0.20136 factor:1 | 1 (-3.28216) | -1 | -1 |
| G: -7130.57649 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -13398.31534 HOMO: -7.33347 LUMO: 0.12789 factor:1 | 1 (-3.37315) | 1 | 1 |
| G: -7130.57649 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -13397.52795 HOMO: -6.70489 LUMO: -0.52518 factor:1 | 1 (-2.58576) | -1 | -1 |
| G: -7130.57649 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -13399.15884 HOMO: -7.25183 LUMO: 0.32109 factor:1 | 1 (-4.21665) | 1 | 1 |
| G: -7130.57649 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -13398.89959 HOMO: -7.29265 LUMO: 0.28028 factor:1 | 1 (-3.95741) | 1 | 1 |
| G: -7130.57649 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -13398.29156 HOMO: -6.57155 LUMO: -0.51702 factor:1 | 1 (-3.34937) | -1 | -1 |
| G: -7130.57649 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -13398.13637 HOMO: -7.08040 LUMO: 0.39729 factor:1 | 1 (-3.19418) | 1 | 1 |
| G: -7130.57649 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -13398.28886 HOMO: -6.24501 LUMO: -0.44627 factor:1 | 1 (-3.34667) | -1 | -1 |
| G: -7130.57649 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -13398.56351 HOMO: -6.73754 LUMO: -0.45443 factor:1 | 1 (-3.62132) | -1 | -1 |
| G: -7130.57649 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -13397.65070 HOMO: -6.24501 LUMO: 0.38096 factor:1 | 1 (-2.70851) | -1 | -1 |
| G: -7130.57649 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -13398.10970 HOMO: -6.86815 LUMO: -0.91974 factor:1 | 1 (-3.16751) | -1 | -1 |
| G: -7130.57649 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -13398.44993 HOMO: -7.40150 LUMO: 0.36191 factor:1 | 1 (-3.50774) | 1 | 1 |
| G: -7130.57649 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -13398.20206 HOMO: -6.44094 LUMO: -0.64219 factor:1 | 1 (-3.25987) | -1 | -1 |
| G: -7130.57649 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -13398.97334 HOMO: -6.69944 LUMO: -0.80001 factor:1 | 1 (-4.03115) | -1 | -1 |
| G: -7130.57649 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -13397.94513 HOMO: -6.61509 LUMO: -0.70750 factor:1 | 1 (-3.00294) | -1 | -1 |
| G: -7130.57649 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -13397.22386 HOMO: -7.52123 LUMO: 0.06803 factor:1 | 1 (-2.28167) | 1 | 1 |
| G: -7130.57649 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -13398.72492 HOMO: -7.34163 LUMO: 0.30477 factor:1 | 1 (-3.78274) | 1 | 1 |
| G: -7130.57649 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -13398.57763 HOMO: -6.68584 LUMO: -0.78641 factor:1 | 1 (-3.63544) | -1 | -1 |
| G: -7130.57649 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -13398.58560 HOMO: -6.53890 LUMO: -0.50885 factor:1 | 1 (-3.64341) | -1 | -1 |
| G: -7130.57649 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -13397.88053 HOMO: -6.75659 LUMO: -0.68845 factor:1 | 1 (-2.93834) | -1 | -1 |
| G: -7130.57649 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -13398.30851 HOMO: -7.08857 LUMO: 0.43266 factor:1 | 1 (-3.36632) | 1 | 1 |
| G: -7130.57649 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -13397.41080 HOMO: -6.28583 LUMO: -0.46804 factor:1 | 1 (-2.46862) | -1 | -1 |
| G: -7130.57649 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -13398.24638 HOMO: -6.50080 LUMO: -0.24762 factor:1 | 1 (-3.30420) | -1 | -1 |
| G: -7130.57649 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -13397.49394 HOMO: -6.45454 LUMO: -0.58504 factor:1 | 1 (-2.55175) | -1 | -1 |
| G: -7130.57649 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -13397.24775 HOMO: -7.20558 LUMO: 0.20953 factor:1 | 1 (-2.30557) | 1 | 1 |
| G: -7130.57649 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -13396.77931 HOMO: -6.35930 LUMO: -0.20681 factor:1 | 1 (-1.83712) | -1 | -1 |
| G: -7130.57649 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -13395.65924 HOMO: -6.36202 LUMO: -0.14422 factor:1 | 1 (-0.71705) | -1 | -1 |
| G: -7130.57649 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -13396.77907 HOMO: -6.20692 LUMO: 1.97827 factor:1 | 1 (-1.83688) | -1 | -1 |
| G: -7130.57649 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -13396.67123 HOMO: -6.48719 LUMO: 1.74153 factor:1 | 1 (-1.72904) | -1 | -1 |
| G: -7130.57649 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -13397.89939 HOMO: -6.84638 LUMO: 1.88575 factor:1 | 1 (-2.95720) | -1 | -1 |
| G: -7130.57649 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -13396.42319 HOMO: -5.90759 LUMO: 2.00820 factor:1 | 1 (-1.48101) | -1 | -1 |
| G: -7130.57649 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -13397.24762 HOMO: -6.56339 LUMO: 1.99732 factor:1 | 1 (-2.30543) | -1 | -1 |
| G: -7130.57649 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -13398.50193 HOMO: -6.20692 LUMO: 1.75241 factor:1 | 1 (-3.55974) | -1 | -1 |
| G: -7130.57649 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -13397.89939 HOMO: -6.16882 LUMO: 1.94017 factor:1 | 1 (-2.95720) | -1 | -1 |
| G: -7130.57649 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -13398.61341 HOMO: -6.80829 LUMO: 1.78507 factor:1 | 1 (-3.67122) | -1 | -1 |
| G: -7130.57649 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -13398.22584 HOMO: -6.58243 LUMO: 1.78235 factor:1 | 1 (-3.28365) | -1 | -1 |
| G: -7130.57649 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -13398.23071 HOMO: -5.85045 LUMO: 1.82316 factor:1 | 1 (-3.28852) | -1 | -1 |
| G: -7130.57649 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -13398.93938 HOMO: -5.93752 LUMO: 1.56465 factor:1 | 1 (-3.99719) | -1 | -1 |
| G: -7130.57649 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -13398.65524 HOMO: -6.59604 LUMO: -0.53334 factor:1 | 1 (-3.71305) | -1 | -1 |
| G: -7130.57649 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -13398.65102 HOMO: -7.06135 LUMO: 0.29660 factor:1 | 1 (-3.70883) | 1 | 1 |
| G: -7130.57649 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -13397.40740 HOMO: -6.50352 LUMO: 1.61908 factor:1 | 1 (-2.46522) | -1 | -1 |
| G: -7130.57649 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -13397.83568 HOMO: -6.68040 LUMO: -0.60681 factor:1 | 1 (-2.89350) | -1 | -1 |
| G: -7130.57649 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -13397.79854 HOMO: -6.93618 LUMO: -1.09662 factor:1 | 1 (-2.85635) | -1 | -1 |
| G: -7130.57649 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -13398.25847 HOMO: -6.72121 LUMO: -1.14016 factor:1 | 1 (-3.31628) | -1 | -1 |
| G: -7130.57649 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -13397.78733 HOMO: -7.12394 LUMO: -1.24900 factor:1 | 1 (-2.84514) | -1 | -1 |
| G: -7130.57649 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -13397.40808 HOMO: -6.71305 LUMO: -0.71566 factor:1 | 1 (-2.46590) | -1 | -1 |
| G: -7130.57649 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -13396.42319 HOMO: -7.09401 LUMO: -0.86532 factor:1 | 1 (-1.48101) | -1 | -1 |
| G: -7130.57649 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -13398.64816 HOMO: -7.08584 LUMO: -0.92519 factor:1 | 1 (-3.70597) | -1 | -1 |
| G: -7130.57649 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -13398.71622 HOMO: -7.05591 LUMO: 0.11973 factor:1 | 1 (-3.77403) | -1 | -1 |
| G: -7130.57649 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -13397.91457 HOMO: -7.14843 LUMO: -1.58370 factor:1 | 1 (-2.97238) | -1 | -1 |
| G: -7130.57649 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -13398.63518 HOMO: -7.36884 LUMO: -1.97010 factor:1 | 1 (-3.69299) | -1 | -1 |
| G: -7130.57649 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -13398.76857 HOMO: -6.81373 LUMO: -1.72248 factor:1 | 1 (-3.82638) | -1 | -1 |
| G: -7130.57649 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -13398.42666 HOMO: -6.87360 LUMO: -1.03947 factor:1 | 1 (-3.48447) | -1 | -1 |
| G: -7130.57649 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -13398.07871 HOMO: -7.02870 LUMO: -0.87349 factor:1 | 1 (-3.13652) | -1 | -1 |
| G: -7130.57649 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -13397.85748 HOMO: -7.16476 LUMO: -1.18097 factor:1 | 1 (-2.91529) | -1 | -1 |
| G: -7130.57649 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -13398.10780 HOMO: -7.51851 LUMO: 0.07891 factor:1 | 1 (-3.16561) | 1 | 1 |
| G: -7130.57649 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -13397.72915 HOMO: -7.04231 LUMO: -0.83539 factor:1 | 1 (-2.78696) | -1 | -1 |
| G: -7130.57649 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -13398.19961 HOMO: -6.83278 LUMO: -0.60137 factor:1 | 1 (-3.25742) | -1 | -1 |
| G: -7130.57649 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -13397.85362 HOMO: -6.89809 LUMO: -1.19186 factor:1 | 1 (-2.91143) | -1 | -1 |
| G: -7130.57649 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -13397.77952 HOMO: -7.16476 LUMO: -0.79185 factor:1 | 1 (-2.83733) | -1 | -1 |
| G: -7130.57649 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -13398.08214 HOMO: -6.97156 LUMO: -1.25444 factor:1 | 1 (-3.13995) | -1 | -1 |
| G: -7130.57649 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -13398.48185 HOMO: -6.84366 LUMO: -0.88437 factor:1 | 1 (-3.53966) | -1 | -1 |
| G: -7130.57649 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -13398.60884 HOMO: -6.91986 LUMO: -1.12655 factor:1 | 1 (-3.66665) | -1 | -1 |
| G: -7130.57649 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -13397.91457 HOMO: -6.49536 LUMO: -0.29660 factor:1 | 1 (-2.97238) | -1 | -1 |
| G: -7130.57649 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -13397.72923 HOMO: -6.74842 LUMO: 0.42450 factor:1 | 1 (-2.78704) | -1 | -1 |
| G: -7130.57649 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -13396.86173 HOMO: -7.34435 LUMO: 0.32109 factor:1 | 1 (-1.91955) | 1 | 1 |
| G: -7130.57649 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -13397.57026 HOMO: -7.16476 LUMO: 0.28572 factor:1 | 1 (-2.62808) | 1 | 1 |
| G: -7130.57649 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -13397.01518 HOMO: -6.74298 LUMO: -0.43538 factor:1 | 1 (-2.07299) | -1 | -1 |
| G: -7130.57649 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -13397.26961 HOMO: -7.19469 LUMO: -1.61091 factor:1 | 1 (-2.32742) | -1 | -1 |
| G: -7130.57649 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -13397.43736 HOMO: -7.35252 LUMO: -1.78235 factor:1 | 1 (-2.49518) | -1 | -1 |
| G: -7130.57649 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -13396.47419 HOMO: -7.25456 LUMO: -1.66806 factor:1 | 1 (-1.53200) | -1 | -1 |
| G: -7130.57649 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -13397.81155 HOMO: -7.54844 LUMO: -1.07213 factor:1 | 1 (-2.86936) | -1 | -1 |
| G: -7130.57649 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -13398.11313 HOMO: -7.21918 LUMO: -1.55377 factor:1 | 1 (-3.17094) | -1 | -1 |
| G: -7130.57649 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -13397.21943 HOMO: -7.01782 LUMO: -1.60547 factor:1 | 1 (-2.27724) | -1 | -1 |
| G: -7130.57649 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -13397.35301 HOMO: -7.21646 LUMO: -1.53472 factor:1 | 1 (-2.41082) | -1 | -1 |
| G: -7130.57649 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -13397.50643 HOMO: -6.73754 LUMO: -1.37417 factor:1 | 1 (-2.56424) | -1 | -1 |
| G: -7130.57649 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -13396.47416 HOMO: -6.78924 LUMO: 0.66396 factor:1 | 1 (-1.53197) | -1 | -1 |
| G: -7130.57649 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -13398.90316 HOMO: -6.82734 LUMO: 0.61226 factor:1 | 1 (-3.96097) | -1 | -1 |
| G: -7130.57649 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -13397.48400 HOMO: -6.74026 LUMO: 0.65579 factor:1 | 1 (-2.54182) | -1 | -1 |
| G: -7130.57649 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -13398.03463 HOMO: -7.10489 LUMO: -1.30887 factor:1 | 1 (-3.09244) | -1 | -1 |
| G: -7130.57649 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -13398.28122 HOMO: -7.05047 LUMO: 0.42722 factor:1 | 1 (-3.33903) | -1 | -1 |
| G: -7130.57649 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -13397.86129 HOMO: -6.61237 LUMO: 1.30887 factor:1 | 1 (-2.91910) | -1 | -1 |
| G: -7130.57649 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -13398.18513 HOMO: -7.05863 LUMO: 0.59049 factor:1 | 1 (-3.24294) | -1 | -1 |
| G: -7130.57649 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -13397.71081 HOMO: -6.26406 LUMO: 0.78641 factor:1 | 1 (-2.76862) | -1 | -1 |
| G: -7130.57649 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -13397.51053 HOMO: -6.70489 LUMO: 0.67756 factor:1 | 1 (-2.56835) | -1 | -1 |
| G: -7130.57649 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -13398.42707 HOMO: -6.78652 LUMO: -0.94968 factor:1 | 1 (-3.48488) | -1 | -1 |
| G: -7130.57649 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -13397.07942 HOMO: -6.36202 LUMO: -0.94424 factor:1 | 1 (-2.13724) | -1 | -1 |
| G: -7130.57649 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -13397.60414 HOMO: -6.81645 LUMO: -1.09934 factor:1 | 1 (-2.66195) | -1 | -1 |
| G: -7130.57649 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -13397.98415 HOMO: -7.07224 LUMO: 0.85988 factor:1 | 1 (-3.04196) | 1 | 1 |
| G: -7130.57649 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -13397.65078 HOMO: -7.02326 LUMO: 1.10206 factor:1 | 1 (-2.70859) | -1 | -1 |
| G: -7130.57649 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -13397.28256 HOMO: -6.71305 LUMO: 0.84627 factor:1 | 1 (-2.34037) | -1 | -1 |
| G: -7130.57649 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -13397.44749 HOMO: -7.27360 LUMO: 0.88165 factor:1 | 1 (-2.50530) | 1 | 1 |