乙二醇作为反应物的反应表19-16

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: -5683.64846 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.41495 HOMO: -6.91169 LUMO: -0.53879 factor:1 | 1 (-0.40080) | -1 | -1 |
| G: -5683.64846 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.09308 HOMO: -7.29809 LUMO: 2.83543 factor:1 | 1 (-1.07893) | 1 | -1 |
| G: -5683.64846 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.32348 HOMO: -6.86543 LUMO: -0.70205 factor:1 | 1 (-1.30933) | -1 | -1 |
| G: -5683.64846 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.25000 HOMO: -7.47769 LUMO: 0.31293 factor:1 | 1 (-2.23585) | -1 | -1 |
| G: -5683.64846 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.69720 HOMO: -6.63141 LUMO: -0.55511 factor:1 | 1 (-1.68305) | -1 | -1 |
| G: -5683.64846 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.65064 HOMO: -6.68856 LUMO: -0.30205 factor:1 | 1 (-1.63649) | -1 | -1 |
| G: -5683.64846 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.84200 HOMO: -7.22190 LUMO: 0.53334 factor:1 | 1 (-0.82785) | -1 | -1 |
| G: -5683.64846 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.55200 HOMO: -6.66407 LUMO: -0.27756 factor:1 | 1 (-1.53785) | -1 | -1 |
| G: -5683.64846 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11946.83647 HOMO: -7.15659 LUMO: -0.70205 factor:1 | -1 (1.17768) | -1 | -1 |
| G: -5683.64846 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.22480 HOMO: -6.69400 LUMO: 1.67622 factor:1 | 1 (-0.21064) | -1 | -1 |
| G: -5683.64846 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.94901 HOMO: -6.60420 LUMO: 2.16058 factor:1 | -1 (0.06514) | -1 | -1 |
| G: -5683.64846 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.80612 HOMO: -6.87087 LUMO: 1.88031 factor:1 | -1 (0.20803) | -1 | -1 |
| G: -5683.64846 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.89819 HOMO: -6.60965 LUMO: -0.19864 factor:1 | 1 (-1.88403) | -1 | -1 |
| G: -5683.64846 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.71391 HOMO: -7.29265 LUMO: 0.52246 factor:1 | 1 (-1.69976) | -1 | -1 |
| G: -5683.64846 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.47262 HOMO: -6.86543 LUMO: -0.59593 factor:1 | -1 (0.54153) | -1 | -1 |
| G: -5683.64846 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11946.70452 HOMO: -7.44504 LUMO: -1.01226 factor:1 | -1 (1.30963) | -1 | -1 |
| G: -5683.64846 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.15334 HOMO: -6.92530 LUMO: -0.75103 factor:1 | 1 (-0.13919) | -1 | -1 |
| G: -5683.64846 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.61635 HOMO: -7.10489 LUMO: 2.20412 factor:1 | -1 (0.39780) | 1 | 1 |
| G: -5683.64846 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.36639 HOMO: -6.58788 LUMO: 1.73881 factor:1 | 1 (-1.35224) | -1 | -1 |
| G: -5683.64846 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.93990 HOMO: -6.64502 LUMO: 1.70343 factor:1 | 1 (-1.92575) | -1 | -1 |
| G: -5683.64846 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.90905 HOMO: -6.73754 LUMO: 1.60819 factor:1 | 1 (-0.89490) | -1 | -1 |
| G: -5683.64846 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.73500 HOMO: -6.80829 LUMO: 2.45991 factor:1 | 1 (-1.72085) | -1 | -1 |
| G: -5683.64846 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.96677 HOMO: -6.91713 LUMO: 2.43814 factor:1 | 1 (-0.95262) | -1 | -1 |
| G: -5683.64846 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.76510 HOMO: -6.60692 LUMO: 1.93745 factor:1 | 1 (-0.75095) | -1 | -1 |
| G: -5683.64846 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.61914 HOMO: -6.26134 LUMO: 1.46125 factor:1 | 1 (-0.60499) | -1 | -1 |
| G: -5683.64846 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.48408 HOMO: -7.54028 LUMO: 0.25851 factor:1 | 1 (-1.46993) | -1 | -1 |
| G: -5683.64846 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.35865 HOMO: -6.97700 LUMO: -0.73471 factor:1 | 1 (-0.34450) | -1 | -1 |
| G: -5683.64846 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.70394 HOMO: -6.92258 LUMO: -0.70205 factor:1 | -1 (0.31021) | -1 | -1 |
| G: -5683.64846 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.77877 HOMO: -6.83550 LUMO: -0.56872 factor:1 | -1 (0.23538) | -1 | -1 |
| G: -5683.64846 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.68726 HOMO: -6.72121 LUMO: 1.89663 factor:1 | -1 (0.32689) | -1 | -1 |
| G: -5683.64846 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.69715 HOMO: -6.73482 LUMO: 1.89935 factor:1 | 1 (-1.68300) | -1 | -1 |
| G: -5683.64846 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.96121 HOMO: -6.61781 LUMO: 1.86670 factor:1 | 1 (-1.94706) | -1 | -1 |
| G: -5683.64846 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.28849 HOMO: -7.01782 LUMO: 2.26399 factor:1 | 1 (-1.27434) | -1 | -1 |
| G: -5683.64846 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.08095 HOMO: -7.23551 LUMO: 2.09800 factor:1 | 1 (-1.06680) | 1 | 1 |
| G: -5683.64846 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.92918 HOMO: -7.13483 LUMO: 2.17963 factor:1 | 1 (-1.91503) | 1 | 1 |
| G: -5683.64846 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.83348 HOMO: -6.22869 LUMO: 2.01092 factor:1 | 1 (-1.81933) | -1 | -1 |
| G: -5683.64846 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.67399 HOMO: -6.80285 LUMO: 2.14970 factor:1 | 1 (-1.65984) | -1 | -1 |
| G: -5683.64846 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.21649 HOMO: -7.21102 LUMO: 2.33746 factor:1 | 1 (-1.20234) | 1 | 1 |
| G: -5683.64846 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.63214 HOMO: -6.39740 LUMO: 2.59597 factor:1 | 1 (-1.61799) | -1 | -1 |
| G: -5683.64846 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.84170 HOMO: -7.07768 LUMO: 2.48168 factor:1 | 1 (-1.82754) | 1 | 1 |
| G: -5683.64846 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.91697 HOMO: -7.11306 LUMO: 0.90614 factor:1 | 1 (-0.90282) | -1 | -1 |
| G: -5683.64846 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.86677 HOMO: -6.61781 LUMO: -2.46263 factor:1 | 1 (-0.85261) | -1 | -1 |
| G: -5683.64846 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.84549 HOMO: -6.96611 LUMO: 0.90614 factor:1 | 1 (-0.83134) | -1 | -1 |
| G: -5683.64846 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.74992 HOMO: -6.86271 LUMO: -1.14832 factor:1 | 1 (-0.73577) | -1 | -1 |
| G: -5683.64846 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.80442 HOMO: -6.72665 LUMO: 0.96873 factor:1 | 1 (-0.79027) | -1 | -1 |
| G: -5683.64846 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.60839 HOMO: -7.14571 LUMO: 1.05036 factor:1 | 1 (-0.59424) | -1 | -1 |
| G: -5683.64846 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.07977 HOMO: -7.14299 LUMO: 0.98777 factor:1 | 1 (-2.06562) | -1 | -1 |
| G: -5683.64846 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.63334 HOMO: -6.99333 LUMO: 1.05852 factor:1 | 1 (-1.61919) | -1 | -1 |
| G: -5683.64846 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.83224 HOMO: -6.78924 LUMO: -1.49935 factor:1 | 1 (-2.81809) | -1 | -1 |
| G: -5683.64846 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.62687 HOMO: -7.13755 LUMO: 0.94151 factor:1 | 1 (-0.61272) | -1 | -1 |
| G: -5683.64846 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.22250 HOMO: -6.72938 LUMO: -0.35375 factor:1 | 1 (-1.20835) | -1 | -1 |
| G: -5683.64846 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.23066 HOMO: -6.99061 LUMO: 0.82450 factor:1 | 1 (-1.21651) | -1 | -1 |
| G: -5683.64846 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.78704 HOMO: -6.75114 LUMO: -0.68028 factor:1 | 1 (-0.77288) | -1 | -1 |
| G: -5683.64846 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.65957 HOMO: -6.40556 LUMO: -0.42722 factor:1 | 1 (-1.64542) | -1 | -1 |
| G: -5683.64846 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.86028 HOMO: -7.18653 LUMO: 0.42178 factor:1 | 1 (-1.84613) | -1 | -1 |
| G: -5683.64846 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.52218 HOMO: -6.63958 LUMO: -0.71294 factor:1 | 1 (-1.50803) | -1 | -1 |
| G: -5683.64846 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.53076 HOMO: -6.63958 LUMO: -0.71022 factor:1 | 1 (-0.51661) | -1 | -1 |
| G: -5683.64846 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.75340 HOMO: -6.69672 LUMO: -0.72654 factor:1 | 1 (-0.73925) | -1 | -1 |
| G: -5683.64846 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.74176 HOMO: -6.56883 LUMO: -0.80274 factor:1 | 1 (-0.72761) | -1 | -1 |
| G: -5683.64846 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.43849 HOMO: -6.68584 LUMO: -0.56872 factor:1 | 1 (-0.42433) | -1 | -1 |
| G: -5683.64846 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.77792 HOMO: -6.59060 LUMO: -0.35647 factor:1 | 1 (-0.76377) | -1 | -1 |
| G: -5683.64846 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.68521 HOMO: -6.72121 LUMO: -0.71838 factor:1 | 1 (-0.67106) | -1 | -1 |
| G: -5683.64846 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.35340 HOMO: -6.57971 LUMO: -0.61498 factor:1 | 1 (-0.33924) | -1 | -1 |
| G: -5683.64846 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.69381 HOMO: -7.07496 LUMO: 0.50613 factor:1 | 1 (-0.67966) | -1 | -1 |
| G: -5683.64846 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.51683 HOMO: -7.14027 LUMO: 0.43266 factor:1 | 1 (-0.50268) | -1 | -1 |
| G: -5683.64846 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.65266 HOMO: -6.43277 LUMO: -0.44082 factor:1 | 1 (-1.63851) | -1 | -1 |
| G: -5683.64846 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.57764 HOMO: -6.79468 LUMO: 0.07619 factor:1 | 1 (-1.56348) | -1 | -1 |
| G: -5683.64846 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.79006 HOMO: -6.81917 LUMO: -2.57148 factor:1 | 1 (-0.77591) | -1 | -1 |
| G: -5683.64846 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.89341 HOMO: -6.71849 LUMO: 1.30615 factor:1 | -1 (0.12074) | -1 | -1 |
| G: -5683.64846 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.30056 HOMO: -6.85455 LUMO: -0.63675 factor:1 | 1 (-2.28641) | -1 | -1 |
| G: -5683.64846 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.19267 HOMO: -6.73210 LUMO: -1.03131 factor:1 | 1 (-2.17852) | -1 | -1 |
| G: -5683.64846 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.89417 HOMO: -6.83550 LUMO: -0.58777 factor:1 | 1 (-0.88002) | -1 | -1 |
| G: -5683.64846 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.83901 HOMO: -6.53073 LUMO: -0.74287 factor:1 | 1 (-0.82486) | -1 | -1 |
| G: -5683.64846 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.68009 HOMO: -7.18381 LUMO: -0.92791 factor:1 | 1 (-1.66594) | -1 | -1 |
| G: -5683.64846 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.19798 HOMO: -6.49264 LUMO: -0.44627 factor:1 | 1 (-1.18383) | -1 | -1 |
| G: -5683.64846 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.11219 HOMO: -7.32803 LUMO: 0.41361 factor:1 | 1 (-1.09803) | -1 | -1 |
| G: -5683.64846 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.34752 HOMO: -6.53073 LUMO: -0.52790 factor:1 | 1 (-0.33337) | -1 | -1 |
| G: -5683.64846 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.73085 HOMO: -6.54978 LUMO: -0.53062 factor:1 | 1 (-0.71669) | -1 | -1 |
| G: -5683.64846 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.39222 HOMO: -6.56611 LUMO: -0.37824 factor:1 | 1 (-1.37807) | -1 | -1 |
| G: -5683.64846 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.36492 HOMO: -6.57155 LUMO: -0.64219 factor:1 | 1 (-2.35076) | -1 | -1 |
| G: -5683.64846 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.73617 HOMO: -7.08040 LUMO: 0.45715 factor:1 | 1 (-1.72202) | -1 | -1 |
| G: -5683.64846 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.20730 HOMO: -6.66679 LUMO: -0.75376 factor:1 | 1 (-0.19315) | -1 | -1 |
| G: -5683.64846 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.00205 HOMO: -6.83550 LUMO: -0.99322 factor:1 | 1 (-1.98790) | -1 | -1 |
| G: -5683.64846 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.03455 HOMO: -6.53345 LUMO: -0.29660 factor:1 | 1 (-1.02040) | -1 | -1 |
| G: -5683.64846 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.71205 HOMO: -6.65046 LUMO: 2.40549 factor:1 | 1 (-2.69790) | -1 | -1 |
| G: -5683.64846 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.54041 HOMO: -6.98788 LUMO: 2.01092 factor:1 | 1 (-1.52626) | -1 | -1 |
| G: -5683.64846 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.93711 HOMO: -6.61781 LUMO: 1.92384 factor:1 | 1 (-0.92296) | -1 | -1 |
| G: -5683.64846 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.59486 HOMO: -6.61237 LUMO: 2.06807 factor:1 | 1 (-1.58071) | -1 | -1 |
| G: -5683.64846 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.76140 HOMO: -6.59060 LUMO: 1.95106 factor:1 | 1 (-0.74725) | -1 | -1 |
| G: -5683.64846 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.03910 HOMO: -6.48175 LUMO: 1.72248 factor:1 | 1 (-1.02494) | -1 | -1 |
| G: -5683.64846 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.10204 HOMO: -6.84911 LUMO: 2.03541 factor:1 | 1 (-1.08788) | -1 | -1 |
| G: -5683.64846 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.34931 HOMO: -6.50624 LUMO: 2.17147 factor:1 | 1 (-0.33516) | -1 | -1 |
| G: -5683.64846 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.61495 HOMO: -6.68312 LUMO: 2.08439 factor:1 | 1 (-0.60080) | -1 | -1 |
| G: -5683.64846 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.37231 HOMO: -6.96067 LUMO: 1.98099 factor:1 | 1 (-0.35816) | -1 | -1 |
| G: -5683.64846 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.52681 HOMO: -6.93618 LUMO: 1.85854 factor:1 | 1 (-1.51265) | -1 | -1 |
| G: -5683.64846 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.22266 HOMO: -6.71305 LUMO: -0.61226 factor:1 | 1 (-2.20850) | -1 | -1 |
| G: -5683.64846 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.70210 HOMO: -7.06408 LUMO: 0.80001 factor:1 | 1 (-1.68795) | -1 | -1 |
| G: -5683.64846 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.78440 HOMO: -6.52257 LUMO: 0.99049 factor:1 | 1 (-0.77025) | -1 | -1 |
| G: -5683.64846 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.85358 HOMO: -6.84638 LUMO: 1.10750 factor:1 | -1 (0.16057) | -1 | -1 |
| G: -5683.64846 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.38313 HOMO: -6.85455 LUMO: 0.84900 factor:1 | 1 (-1.36898) | -1 | -1 |
| G: -5683.64846 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.54961 HOMO: -6.60148 LUMO: -0.78369 factor:1 | 1 (-1.53546) | -1 | -1 |
| G: -5683.64846 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.83114 HOMO: -6.86543 LUMO: -0.93063 factor:1 | 1 (-1.81699) | -1 | -1 |
| G: -5683.64846 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.16608 HOMO: -6.70489 LUMO: -0.72382 factor:1 | 1 (-2.15193) | -1 | -1 |
| G: -5683.64846 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.45595 HOMO: -6.59060 LUMO: 0.31293 factor:1 | 1 (-1.44180) | -1 | -1 |
| G: -5683.64846 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.46672 HOMO: -6.52257 LUMO: -0.48708 factor:1 | 1 (-1.45257) | -1 | -1 |
| G: -5683.64846 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.59108 HOMO: -6.54706 LUMO: -0.48164 factor:1 | 1 (-1.57693) | -1 | -1 |
| G: -5683.64846 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.68127 HOMO: -7.32803 LUMO: 0.08436 factor:1 | 1 (-0.66711) | -1 | -1 |
| G: -5683.64846 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.81720 HOMO: -6.77291 LUMO: -0.66940 factor:1 | -1 (0.19696) | -1 | -1 |
| G: -5683.64846 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.22321 HOMO: -6.68312 LUMO: -0.53062 factor:1 | 1 (-1.20906) | -1 | -1 |
| G: -5683.64846 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.55185 HOMO: -7.07768 LUMO: 0.45987 factor:1 | 1 (-0.53770) | -1 | -1 |
| G: -5683.64846 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.38327 HOMO: -6.50352 LUMO: -0.63675 factor:1 | 1 (-0.36912) | -1 | -1 |
| G: -5683.64846 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.12236 HOMO: -6.48992 LUMO: -0.60681 factor:1 | 1 (-1.10821) | -1 | -1 |
| G: -5683.64846 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.27866 HOMO: -6.65318 LUMO: -0.72382 factor:1 | 1 (-2.26450) | -1 | -1 |
| G: -5683.64846 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11951.03755 HOMO: -6.54706 LUMO: 0.24218 factor:1 | 1 (-3.02340) | -1 | -1 |
| G: -5683.64846 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.02935 HOMO: -6.63958 LUMO: 0.57416 factor:1 | 1 (-1.01520) | -1 | -1 |
| G: -5683.64846 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.30065 HOMO: -6.37563 LUMO: -0.48164 factor:1 | 1 (-1.28650) | -1 | -1 |
| G: -5683.64846 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.05884 HOMO: -6.64774 LUMO: -0.71838 factor:1 | 1 (-2.04469) | -1 | -1 |
| G: -5683.64846 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.34356 HOMO: -7.17020 LUMO: 0.45987 factor:1 | 1 (-1.32941) | -1 | -1 |
| G: -5683.64846 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.01544 HOMO: -6.86543 LUMO: -1.05036 factor:1 | 1 (-2.00129) | -1 | -1 |
| G: -5683.64846 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.44330 HOMO: -6.77019 LUMO: -1.03131 factor:1 | 1 (-0.42915) | -1 | -1 |
| G: -5683.64846 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.00568 HOMO: -6.80285 LUMO: 1.05852 factor:1 | 1 (-0.99153) | -1 | -1 |
| G: -5683.64846 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.05642 HOMO: -6.76475 LUMO: 1.01771 factor:1 | -1 (0.95773) | -1 | -1 |
| G: -5683.64846 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11946.39412 HOMO: -6.92530 LUMO: 1.37417 factor:1 | -1 (1.62003) | -1 | -1 |
| G: -5683.64846 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11946.27366 HOMO: -6.98244 LUMO: 1.25989 factor:1 | -1 (1.74049) | -1 | -1 |
| G: -5683.64846 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11946.10865 HOMO: -6.74842 LUMO: 0.89798 factor:1 | -1 (1.90550) | -1 | -1 |
| G: -5683.64846 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11945.95305 HOMO: -6.77019 LUMO: -1.17009 factor:1 | -1 (2.06110) | -1 | -1 |
| G: -5683.64846 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.96048 HOMO: -6.78652 LUMO: 1.35785 factor:1 | 1 (-0.94633) | -1 | -1 |
| G: -5683.64846 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.81414 HOMO: -6.82734 LUMO: -0.68301 factor:1 | 1 (-0.79999) | -1 | -1 |
| G: -5683.64846 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.21290 HOMO: -6.48175 LUMO: -2.19052 factor:1 | 1 (-0.19875) | -1 | -1 |
| G: -5683.64846 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.96685 HOMO: -6.65863 LUMO: -0.77008 factor:1 | 1 (-0.95270) | -1 | -1 |
| G: -5683.64846 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.93893 HOMO: -6.44094 LUMO: -2.20956 factor:1 | 1 (-0.92478) | -1 | -1 |
| G: -5683.64846 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.30262 HOMO: -6.59876 LUMO: -0.57688 factor:1 | 1 (-0.28847) | -1 | -1 |
| G: -5683.64846 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.08616 HOMO: -6.78380 LUMO: -0.77008 factor:1 | 1 (-2.07201) | -1 | -1 |
| G: -5683.64846 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.15959 HOMO: -7.30354 LUMO: 0.25034 factor:1 | 1 (-1.14544) | -1 | -1 |
| G: -5683.64846 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.06721 HOMO: -6.59332 LUMO: -0.53334 factor:1 | 1 (-1.05305) | -1 | -1 |
| G: -5683.64846 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.82910 HOMO: -6.64230 LUMO: -0.55783 factor:1 | 1 (-1.81495) | -1 | -1 |
| G: -5683.64846 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.45639 HOMO: -7.26544 LUMO: 0.20409 factor:1 | 1 (-0.44224) | -1 | -1 |
| G: -5683.64846 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.23397 HOMO: -6.61237 LUMO: -0.65307 factor:1 | -1 (0.78018) | -1 | -1 |
| G: -5683.64846 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11944.11171 HOMO: -6.72393 LUMO: -0.65307 factor:1 | -1 (3.90244) | -1 | -1 |
| G: -5683.64846 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11943.99002 HOMO: -6.29671 LUMO: -0.39729 factor:1 | -1 (4.02413) | -1 | -1 |
| G: -5683.64846 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.55375 HOMO: -6.75387 LUMO: -0.53334 factor:1 | 1 (-0.53960) | -1 | -1 |
| G: -5683.64846 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.81999 HOMO: -6.53073 LUMO: -0.31293 factor:1 | 1 (-0.80584) | -1 | -1 |
| G: -5683.64846 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.26498 HOMO: -6.42189 LUMO: -0.59049 factor:1 | 1 (-1.25083) | -1 | -1 |
| G: -5683.64846 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.07315 HOMO: -6.41100 LUMO: -0.29933 factor:1 | -1 (0.94100) | -1 | -1 |
| G: -5683.64846 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.08461 HOMO: -6.57427 LUMO: -0.53879 factor:1 | -1 (0.92954) | -1 | -1 |
| G: -5683.64846 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11946.13442 HOMO: -7.43143 LUMO: 0.33470 factor:1 | -1 (1.87974) | -1 | -1 |
| G: -5683.64846 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11945.91194 HOMO: -6.56067 LUMO: -0.50885 factor:1 | -1 (2.10222) | -1 | -1 |
| G: -5683.64846 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.60906 HOMO: -6.65863 LUMO: -0.76464 factor:1 | -1 (0.40510) | -1 | -1 |
| G: -5683.64846 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.08760 HOMO: -6.32665 LUMO: -0.41906 factor:1 | -1 (0.92655) | -1 | -1 |
| G: -5683.64846 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.82062 HOMO: -6.57699 LUMO: 1.63813 factor:1 | 1 (-0.80646) | -1 | -1 |
| G: -5683.64846 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11946.77761 HOMO: -6.53073 LUMO: 1.71704 factor:1 | -1 (1.23654) | -1 | -1 |
| G: -5683.64846 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11946.92112 HOMO: -6.86271 LUMO: 2.07351 factor:1 | -1 (1.09303) | -1 | -1 |
| G: -5683.64846 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.76296 HOMO: -6.63686 LUMO: 1.78235 factor:1 | -1 (0.25119) | -1 | -1 |
| G: -5683.64846 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.89722 HOMO: -6.60965 LUMO: 1.94289 factor:1 | -1 (0.11693) | -1 | -1 |
| G: -5683.64846 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.63684 HOMO: -6.55250 LUMO: 1.89119 factor:1 | -1 (0.37731) | -1 | -1 |
| G: -5683.64846 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.84129 HOMO: -6.50624 LUMO: 1.85582 factor:1 | 1 (-1.82714) | -1 | -1 |
| G: -5683.64846 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.10168 HOMO: -6.06814 LUMO: 1.94561 factor:1 | 1 (-1.08753) | -1 | -1 |
| G: -5683.64846 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.88445 HOMO: -6.58788 LUMO: 2.01908 factor:1 | 1 (-0.87030) | -1 | -1 |
| G: -5683.64846 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.15357 HOMO: -6.74026 LUMO: 0.31293 factor:1 | 1 (-1.13942) | -1 | -1 |
| G: -5683.64846 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.19854 HOMO: -6.54434 LUMO: -0.42994 factor:1 | -1 (0.81561) | -1 | -1 |
| G: -5683.64846 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.89362 HOMO: -6.94707 LUMO: 0.42994 factor:1 | 1 (-0.87947) | -1 | -1 |
| G: -5683.64846 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.75169 HOMO: -6.98516 LUMO: 0.41361 factor:1 | 1 (-0.73754) | -1 | -1 |
| G: -5683.64846 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.77533 HOMO: -6.31304 LUMO: -0.54967 factor:1 | 1 (-1.76118) | -1 | -1 |
| G: -5683.64846 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.86591 HOMO: -6.48447 LUMO: -0.40817 factor:1 | 1 (-1.85176) | -1 | -1 |
| G: -5683.64846 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.17406 HOMO: -6.49264 LUMO: 0.29116 factor:1 | 1 (-1.15991) | -1 | -1 |
| G: -5683.64846 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.88358 HOMO: -6.48719 LUMO: -0.11973 factor:1 | 1 (-0.86943) | -1 | -1 |
| G: -5683.64846 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.60894 HOMO: -7.16204 LUMO: 0.44082 factor:1 | 1 (-0.59479) | -1 | -1 |
| G: -5683.64846 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.80668 HOMO: -6.74842 LUMO: -0.37552 factor:1 | 1 (-0.79253) | -1 | -1 |
| G: -5683.64846 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.73489 HOMO: -6.44638 LUMO: -0.45171 factor:1 | 1 (-1.72074) | -1 | -1 |
| G: -5683.64846 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.89982 HOMO: -7.07496 LUMO: 0.50341 factor:1 | 1 (-1.88567) | -1 | -1 |
| G: -5683.64846 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.91043 HOMO: -6.79468 LUMO: 0.11429 factor:1 | 1 (-1.89628) | -1 | -1 |
| G: -5683.64846 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.32834 HOMO: -6.63958 LUMO: -0.67484 factor:1 | 1 (-2.31419) | -1 | -1 |
| G: -5683.64846 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.49451 HOMO: -7.08584 LUMO: 0.46259 factor:1 | 1 (-1.48035) | -1 | -1 |
| G: -5683.64846 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.25944 HOMO: -6.80285 LUMO: -0.73199 factor:1 | 1 (-2.24529) | -1 | -1 |
| G: -5683.64846 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.85396 HOMO: -6.44366 LUMO: -0.45443 factor:1 | 1 (-2.83981) | -1 | -1 |
| G: -5683.64846 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.13521 HOMO: -6.75931 LUMO: 0.25851 factor:1 | 1 (-1.12105) | -1 | -1 |
| G: -5683.64846 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.62325 HOMO: -6.64502 LUMO: 1.79323 factor:1 | 1 (-0.60910) | -1 | -1 |
| G: -5683.64846 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.20680 HOMO: -6.51168 LUMO: 1.60275 factor:1 | 1 (-1.19265) | -1 | -1 |
| G: -5683.64846 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.41762 HOMO: -6.56067 LUMO: 1.63268 factor:1 | 1 (-0.40346) | -1 | -1 |
| G: -5683.64846 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.53959 HOMO: -6.56883 LUMO: 1.70615 factor:1 | 1 (-2.52543) | -1 | -1 |
| G: -5683.64846 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.11318 HOMO: -6.77836 LUMO: 1.77962 factor:1 | 1 (-2.09903) | -1 | -1 |
| G: -5683.64846 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.57930 HOMO: -6.38923 LUMO: 1.85854 factor:1 | 1 (-1.56514) | -1 | -1 |
| G: -5683.64846 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.78270 HOMO: -6.35658 LUMO: 2.16875 factor:1 | 1 (-1.76855) | -1 | -1 |
| G: -5683.64846 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.21543 HOMO: -6.83006 LUMO: 2.31025 factor:1 | 1 (-1.20127) | -1 | -1 |
| G: -5683.64846 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.72335 HOMO: -6.87087 LUMO: 1.79051 factor:1 | 1 (-1.70920) | -1 | -1 |
| G: -5683.64846 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.82246 HOMO: -6.56339 LUMO: 2.37828 factor:1 | 1 (-1.80831) | -1 | -1 |
| G: -5683.64846 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.12274 HOMO: -6.30488 LUMO: 2.51705 factor:1 | 1 (-1.10859) | -1 | -1 |
| G: -5683.64846 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.20609 HOMO: -6.69400 LUMO: 1.95650 factor:1 | 1 (-1.19194) | -1 | -1 |
| G: -5683.64846 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.94705 HOMO: -6.51168 LUMO: 2.03541 factor:1 | 1 (-2.93290) | -1 | -1 |
| G: -5683.64846 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11951.73909 HOMO: -6.30760 LUMO: 1.65173 factor:1 | 1 (-3.72494) | -1 | -1 |
| G: -5683.64846 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.94925 HOMO: -6.55250 LUMO: 1.90752 factor:1 | 1 (-2.93510) | -1 | -1 |
| G: -5683.64846 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11951.13587 HOMO: -6.41372 LUMO: 1.76058 factor:1 | 1 (-3.12172) | -1 | -1 |
| G: -5683.64846 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.48514 HOMO: -6.23957 LUMO: 2.06534 factor:1 | 1 (-2.47098) | -1 | -1 |
| G: -5683.64846 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.60419 HOMO: -6.58243 LUMO: 2.11705 factor:1 | 1 (-2.59003) | -1 | -1 |
| G: -5683.64846 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.78125 HOMO: -6.37835 LUMO: 2.09256 factor:1 | 1 (-2.76710) | -1 | -1 |
| G: -5683.64846 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.46078 HOMO: -6.50624 LUMO: 2.55787 factor:1 | 1 (-2.44663) | -1 | -1 |
| G: -5683.64846 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.10296 HOMO: -6.45454 LUMO: 1.87214 factor:1 | 1 (-1.08881) | -1 | -1 |
| G: -5683.64846 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.45855 HOMO: -6.53617 LUMO: 1.95650 factor:1 | 1 (-2.44440) | -1 | -1 |
| G: -5683.64846 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.05473 HOMO: -6.51985 LUMO: 1.71432 factor:1 | 1 (-2.04058) | -1 | -1 |
| G: -5683.64846 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.05444 HOMO: -6.75114 LUMO: 1.84493 factor:1 | 1 (-1.04029) | -1 | -1 |
| G: -5683.64846 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.12944 HOMO: -6.06270 LUMO: 1.65717 factor:1 | 1 (-1.11529) | -1 | -1 |
| G: -5683.64846 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.43495 HOMO: -5.89671 LUMO: 1.71704 factor:1 | 1 (-0.42080) | -1 | -1 |
| G: -5683.64846 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.12666 HOMO: -6.18787 LUMO: 1.91840 factor:1 | 1 (-1.11251) | -1 | -1 |
| G: -5683.64846 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.80870 HOMO: -6.01644 LUMO: 1.85582 factor:1 | 1 (-0.79455) | -1 | -1 |
| G: -5683.64846 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.26188 HOMO: -6.05998 LUMO: 2.33474 factor:1 | 1 (-1.24772) | -1 | -1 |
| G: -5683.64846 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.30925 HOMO: -6.05725 LUMO: 2.03541 factor:1 | 1 (-1.29510) | -1 | -1 |
| G: -5683.64846 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.65525 HOMO: -6.80829 LUMO: 1.90480 factor:1 | 1 (-0.64110) | -1 | -1 |
| G: -5683.64846 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.24887 HOMO: -6.76475 LUMO: 2.20956 factor:1 | 1 (-1.23472) | -1 | -1 |
| G: -5683.64846 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.62834 HOMO: -6.29944 LUMO: 1.77962 factor:1 | 1 (-0.61419) | -1 | -1 |
| G: -5683.64846 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.31707 HOMO: -6.47359 LUMO: -0.25579 factor:1 | 1 (-0.30292) | -1 | -1 |
| G: -5683.64846 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.00380 HOMO: -6.57699 LUMO: -0.47348 factor:1 | 1 (-0.98965) | -1 | -1 |
| G: -5683.64846 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.37861 HOMO: -7.20830 LUMO: 0.49797 factor:1 | 1 (-1.36446) | -1 | -1 |
| G: -5683.64846 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.02029 HOMO: -7.49402 LUMO: 0.29933 factor:1 | 1 (-1.00614) | -1 | -1 |
| G: -5683.64846 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.48777 HOMO: -6.66679 LUMO: -0.58777 factor:1 | 1 (-0.47361) | -1 | -1 |
| G: -5683.64846 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.13405 HOMO: -6.67767 LUMO: -0.56328 factor:1 | 1 (-0.11989) | -1 | -1 |
| G: -5683.64846 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.34880 HOMO: -7.42871 LUMO: 0.35647 factor:1 | 1 (-0.33465) | -1 | -1 |
| G: -5683.64846 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.39459 HOMO: -6.56067 LUMO: -0.54423 factor:1 | 1 (-0.38044) | -1 | -1 |
| G: -5683.64846 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.68664 HOMO: -6.56339 LUMO: -0.50341 factor:1 | -1 (0.32752) | -1 | -1 |
| G: -5683.64846 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.00353 HOMO: -6.56067 LUMO: -0.48436 factor:1 | 1 (-0.98938) | -1 | -1 |
| G: -5683.64846 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.10051 HOMO: -6.73210 LUMO: 1.75241 factor:1 | 1 (-1.08636) | -1 | -1 |
| G: -5683.64846 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.47375 HOMO: -6.48175 LUMO: 1.91296 factor:1 | 1 (-0.45960) | -1 | -1 |
| G: -5683.64846 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.22598 HOMO: -6.67767 LUMO: 1.70343 factor:1 | 1 (-1.21183) | -1 | -1 |
| G: -5683.64846 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.59463 HOMO: -6.37835 LUMO: 1.96466 factor:1 | 1 (-0.58047) | -1 | -1 |
| G: -5683.64846 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.72864 HOMO: -6.40828 LUMO: 2.10072 factor:1 | 1 (-0.71449) | -1 | -1 |
| G: -5683.64846 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.10759 HOMO: -6.06542 LUMO: 1.92112 factor:1 | 1 (-1.09344) | -1 | -1 |
| G: -5683.64846 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.20397 HOMO: -6.90353 LUMO: 1.83133 factor:1 | 1 (-1.18982) | -1 | -1 |
| G: -5683.64846 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.61264 HOMO: -6.37019 LUMO: 1.92929 factor:1 | 1 (-0.59849) | -1 | -1 |
| G: -5683.64846 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.10577 HOMO: -6.61509 LUMO: 2.11160 factor:1 | 1 (-0.09162) | -1 | -1 |
| G: -5683.64846 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.15851 HOMO: -6.82734 LUMO: 1.77146 factor:1 | 1 (-0.14436) | -1 | -1 |
| G: -5683.64846 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.89927 HOMO: -6.01100 LUMO: 1.89935 factor:1 | -1 (0.11489) | -1 | -1 |
| G: -5683.64846 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.61201 HOMO: -6.49536 LUMO: 1.75241 factor:1 | 1 (-0.59786) | -1 | -1 |
| G: -5683.64846 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.19695 HOMO: -6.34297 LUMO: 1.86398 factor:1 | 1 (-1.18280) | -1 | -1 |
| G: -5683.64846 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.10391 HOMO: -6.53073 LUMO: 1.84493 factor:1 | 1 (-1.08976) | -1 | -1 |
| G: -5683.64846 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.89300 HOMO: -6.53345 LUMO: 2.41093 factor:1 | 1 (-0.87885) | -1 | -1 |
| G: -5683.64846 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.11420 HOMO: -7.01237 LUMO: 2.06262 factor:1 | 1 (-1.10005) | -1 | -1 |
| G: -5683.64846 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.02009 HOMO: -6.17154 LUMO: 1.89119 factor:1 | 1 (-2.00594) | -1 | -1 |
| G: -5683.64846 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.26278 HOMO: -6.08719 LUMO: 1.74425 factor:1 | 1 (-0.24863) | -1 | -1 |
| G: -5683.64846 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.89182 HOMO: -6.69672 LUMO: 1.95106 factor:1 | 1 (-1.87767) | -1 | -1 |
| G: -5683.64846 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.48353 HOMO: -6.58243 LUMO: 2.24766 factor:1 | 1 (-2.46938) | -1 | -1 |
| G: -5683.64846 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.02281 HOMO: -6.74570 LUMO: 2.02181 factor:1 | 1 (-2.00866) | -1 | -1 |
| G: -5683.64846 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.52688 HOMO: -6.53890 LUMO: 1.92929 factor:1 | 1 (-2.51273) | -1 | -1 |
| G: -5683.64846 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.73388 HOMO: -6.03276 LUMO: 1.67078 factor:1 | 1 (-2.71972) | -1 | -1 |
| G: -5683.64846 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.03509 HOMO: -6.67767 LUMO: 2.03541 factor:1 | 1 (-2.02094) | -1 | -1 |
| G: -5683.64846 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.78477 HOMO: -5.98378 LUMO: 1.84221 factor:1 | 1 (-1.77062) | -1 | -1 |
| G: -5683.64846 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.26053 HOMO: -6.07086 LUMO: 2.01908 factor:1 | 1 (-2.24638) | -1 | -1 |
| G: -5683.64846 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.55720 HOMO: -6.29944 LUMO: 1.90208 factor:1 | 1 (-1.54305) | -1 | -1 |
| G: -5683.64846 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.52702 HOMO: -6.75114 LUMO: 1.85854 factor:1 | 1 (-1.51287) | -1 | -1 |
| G: -5683.64846 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.67650 HOMO: -6.56611 LUMO: 2.49801 factor:1 | 1 (-1.66234) | -1 | -1 |
| G: -5683.64846 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.45633 HOMO: -6.39740 LUMO: 1.92929 factor:1 | 1 (-1.44218) | -1 | -1 |
| G: -5683.64846 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.90257 HOMO: -6.85999 LUMO: -1.07757 factor:1 | 1 (-1.88842) | -1 | -1 |
| G: -5683.64846 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.98367 HOMO: -6.98244 LUMO: 1.07213 factor:1 | 1 (-0.96951) | -1 | -1 |
| G: -5683.64846 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.10187 HOMO: -7.04231 LUMO: 0.64219 factor:1 | 1 (-1.08772) | -1 | -1 |
| G: -5683.64846 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.97866 HOMO: -6.96339 LUMO: 0.75648 factor:1 | 1 (-0.96451) | -1 | -1 |
| G: -5683.64846 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.90897 HOMO: -6.83822 LUMO: -0.97417 factor:1 | 1 (-0.89482) | -1 | -1 |
| G: -5683.64846 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.86268 HOMO: -6.44910 LUMO: -2.15242 factor:1 | 1 (-1.84852) | -1 | -1 |
| G: -5683.64846 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.03759 HOMO: -6.84094 LUMO: -1.37690 factor:1 | 1 (-2.02344) | -1 | -1 |
| G: -5683.64846 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.50365 HOMO: -6.74026 LUMO: -2.54699 factor:1 | 1 (-1.48950) | -1 | -1 |
| G: -5683.64846 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.49187 HOMO: -6.96611 LUMO: 1.24900 factor:1 | 1 (-1.47771) | -1 | -1 |
| G: -5683.64846 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.48234 HOMO: -7.21102 LUMO: 0.82995 factor:1 | 1 (-1.46819) | -1 | -1 |
| G: -5683.64846 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11945.94878 HOMO: -6.88448 LUMO: 0.81634 factor:1 | -1 (2.06537) | -1 | -1 |
| G: -5683.64846 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11946.65026 HOMO: -7.04231 LUMO: 1.10750 factor:1 | -1 (1.36389) | -1 | -1 |
| G: -5683.64846 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.55173 HOMO: -6.83550 LUMO: -0.98777 factor:1 | 1 (-1.53758) | -1 | -1 |
| G: -5683.64846 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.72191 HOMO: -6.82189 LUMO: 0.93879 factor:1 | 1 (-1.70776) | -1 | -1 |
| G: -5683.64846 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.52599 HOMO: -6.81101 LUMO: 0.70750 factor:1 | 1 (-1.51184) | -1 | -1 |
| G: -5683.64846 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.51789 HOMO: -7.06680 LUMO: 0.74015 factor:1 | 1 (-0.50374) | -1 | -1 |
| G: -5683.64846 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.06051 HOMO: -6.68856 LUMO: 0.86260 factor:1 | 1 (-1.04636) | -1 | -1 |
| G: -5683.64846 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.18960 HOMO: -6.83822 LUMO: -0.63403 factor:1 | 1 (-1.17545) | -1 | -1 |
| G: -5683.64846 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.29171 HOMO: -6.84911 LUMO: 1.26533 factor:1 | 1 (-0.27756) | -1 | -1 |
| G: -5683.64846 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.84154 HOMO: -7.01237 LUMO: 0.73743 factor:1 | 1 (-0.82739) | -1 | -1 |
| G: -5683.64846 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.78646 HOMO: -7.00965 LUMO: 1.40139 factor:1 | 1 (-1.77230) | -1 | -1 |
| G: -5683.64846 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.01496 HOMO: -6.73210 LUMO: -2.49256 factor:1 | 1 (-1.00081) | -1 | -1 |
| G: -5683.64846 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.93256 HOMO: -7.08040 LUMO: 0.84627 factor:1 | 1 (-0.91841) | -1 | -1 |
| G: -5683.64846 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.61701 HOMO: -7.00965 LUMO: 0.82995 factor:1 | 1 (-1.60286) | -1 | -1 |
| G: -5683.64846 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.12182 HOMO: -6.88448 LUMO: 0.82723 factor:1 | 1 (-1.10767) | -1 | -1 |
| G: -5683.64846 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.02798 HOMO: -7.20013 LUMO: 0.88437 factor:1 | 1 (-0.01382) | -1 | -1 |
| G: -5683.64846 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.26232 HOMO: -6.60420 LUMO: -0.53334 factor:1 | 1 (-0.24817) | -1 | -1 |
| G: -5683.64846 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.34257 HOMO: -6.78652 LUMO: -0.79729 factor:1 | 1 (-0.32841) | -1 | -1 |
| G: -5683.64846 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.32398 HOMO: -6.48992 LUMO: -0.64491 factor:1 | 1 (-0.30983) | -1 | -1 |
| G: -5683.64846 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.51038 HOMO: -6.85999 LUMO: -0.78097 factor:1 | 1 (-0.49623) | -1 | -1 |
| G: -5683.64846 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.55791 HOMO: -6.65046 LUMO: -0.78097 factor:1 | 1 (-1.54376) | -1 | -1 |
| G: -5683.64846 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.22007 HOMO: -7.24095 LUMO: 0.37280 factor:1 | 1 (-2.20592) | -1 | -1 |
| G: -5683.64846 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.84262 HOMO: -6.81101 LUMO: -0.74831 factor:1 | 1 (-1.82847) | -1 | -1 |
| G: -5683.64846 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.10838 HOMO: -6.69400 LUMO: -0.77280 factor:1 | 1 (-1.09422) | -1 | -1 |
| G: -5683.64846 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.76107 HOMO: -6.08447 LUMO: -0.68573 factor:1 | 1 (-1.74692) | -1 | -1 |
| G: -5683.64846 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.74638 HOMO: -6.66679 LUMO: -0.47076 factor:1 | 1 (-0.73223) | -1 | -1 |
| G: -5683.64846 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.89271 HOMO: -6.97428 LUMO: -1.10750 factor:1 | -1 (0.12144) | -1 | -1 |
| G: -5683.64846 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.88294 HOMO: -6.69128 LUMO: -0.54151 factor:1 | -1 (0.13121) | -1 | -1 |
| G: -5683.64846 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.94650 HOMO: -6.53617 LUMO: -0.35375 factor:1 | -1 (0.06765) | -1 | -1 |
| G: -5683.64846 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.96522 HOMO: -6.75659 LUMO: -0.41361 factor:1 | 1 (-0.95107) | -1 | -1 |
| G: -5683.64846 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.03673 HOMO: -6.69400 LUMO: -0.67484 factor:1 | 1 (-1.02258) | -1 | -1 |
| G: -5683.64846 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.13970 HOMO: -6.89264 LUMO: -0.90886 factor:1 | 1 (-1.12554) | -1 | -1 |
| G: -5683.64846 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.50964 HOMO: -6.56339 LUMO: -0.52518 factor:1 | 1 (-0.49549) | -1 | -1 |
| G: -5683.64846 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.13289 HOMO: -6.45726 LUMO: -0.65852 factor:1 | 1 (-1.11874) | -1 | -1 |
| G: -5683.64846 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.52434 HOMO: -6.80557 LUMO: -0.56600 factor:1 | 1 (-0.51019) | -1 | -1 |
| G: -5683.64846 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.12353 HOMO: -7.19469 LUMO: -0.91702 factor:1 | 1 (-1.10938) | -1 | -1 |
| G: -5683.64846 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.78122 HOMO: -6.41100 LUMO: 0.79185 factor:1 | -1 (0.23293) | -1 | -1 |
| G: -5683.64846 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.23731 HOMO: -6.39195 LUMO: 0.26123 factor:1 | 1 (-0.22316) | -1 | -1 |
| G: -5683.64846 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.95663 HOMO: -6.78924 LUMO: 0.35919 factor:1 | -1 (0.05752) | -1 | -1 |
| G: -5683.64846 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.24792 HOMO: -6.50624 LUMO: 0.71838 factor:1 | 1 (-0.23377) | -1 | -1 |
| G: -5683.64846 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.00340 HOMO: -6.68584 LUMO: -0.66124 factor:1 | -1 (0.01075) | -1 | -1 |
| G: -5683.64846 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.86369 HOMO: -6.45182 LUMO: -0.48980 factor:1 | 1 (-0.84954) | -1 | -1 |
| G: -5683.64846 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.83528 HOMO: -7.18925 LUMO: -1.01498 factor:1 | 1 (-0.82113) | -1 | -1 |
| G: -5683.64846 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.99510 HOMO: -7.18925 LUMO: -0.63130 factor:1 | 1 (-0.98094) | -1 | -1 |
| G: -5683.64846 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.16596 HOMO: -6.66679 LUMO: -0.57960 factor:1 | 1 (-0.15181) | -1 | -1 |
| G: -5683.64846 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.08525 HOMO: -6.44910 LUMO: -0.30205 factor:1 | 1 (-1.07109) | -1 | -1 |
| G: -5683.64846 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.41547 HOMO: -7.23279 LUMO: 0.46804 factor:1 | 1 (-0.40131) | -1 | -1 |
| G: -5683.64846 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.23639 HOMO: -6.92802 LUMO: -0.72927 factor:1 | 1 (-0.22224) | -1 | -1 |
| G: -5683.64846 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.03550 HOMO: -6.83278 LUMO: -0.59321 factor:1 | 1 (-1.02135) | -1 | -1 |
| G: -5683.64846 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.36931 HOMO: -7.44776 LUMO: 0.27211 factor:1 | 1 (-0.35516) | -1 | -1 |
| G: -5683.64846 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.27584 HOMO: -6.80829 LUMO: -0.59865 factor:1 | 1 (-0.26169) | -1 | -1 |
| G: -5683.64846 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.83196 HOMO: -6.63686 LUMO: -0.75103 factor:1 | 1 (-0.81781) | -1 | -1 |
| G: -5683.64846 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.90143 HOMO: -6.73210 LUMO: -0.55511 factor:1 | 1 (-0.88728) | -1 | -1 |
| G: -5683.64846 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.28811 HOMO: -6.50624 LUMO: 1.58642 factor:1 | 1 (-1.27396) | -1 | -1 |
| G: -5683.64846 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.02248 HOMO: -6.79196 LUMO: 0.96328 factor:1 | 1 (-0.00833) | -1 | -1 |
| G: -5683.64846 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.99978 HOMO: -6.82734 LUMO: 1.23540 factor:1 | -1 (0.01437) | -1 | -1 |
| G: -5683.64846 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.01671 HOMO: -6.90081 LUMO: 1.25444 factor:1 | 1 (-0.00256) | -1 | -1 |
| G: -5683.64846 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.05053 HOMO: -7.00965 LUMO: -1.05036 factor:1 | 1 (-0.03638) | -1 | -1 |
| G: -5683.64846 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.87878 HOMO: -7.01237 LUMO: -1.48302 factor:1 | -1 (0.13538) | -1 | -1 |
| G: -5683.64846 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.22659 HOMO: -6.91713 LUMO: 0.93607 factor:1 | 1 (-0.21244) | -1 | -1 |
| G: -5683.64846 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.97845 HOMO: -7.02598 LUMO: 0.92247 factor:1 | -1 (0.03570) | -1 | -1 |
| G: -5683.64846 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.93118 HOMO: -6.98516 LUMO: 1.52384 factor:1 | -1 (0.08297) | -1 | -1 |
| G: -5683.64846 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.94947 HOMO: -6.75387 LUMO: 1.04764 factor:1 | -1 (0.06468) | -1 | -1 |
| G: -5683.64846 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.76912 HOMO: -7.09401 LUMO: 1.19458 factor:1 | 1 (-1.75497) | -1 | -1 |
| G: -5683.64846 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.94435 HOMO: -6.88992 LUMO: -1.56193 factor:1 | 1 (-0.93019) | -1 | -1 |
| G: -5683.64846 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.69898 HOMO: -7.00149 LUMO: 0.99866 factor:1 | 1 (-0.68483) | -1 | -1 |
| G: -5683.64846 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.03365 HOMO: -7.13755 LUMO: 1.05308 factor:1 | 1 (-1.01950) | -1 | -1 |
| G: -5683.64846 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.17448 HOMO: -6.85183 LUMO: -1.42860 factor:1 | 1 (-0.16033) | -1 | -1 |
| G: -5683.64846 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11946.90423 HOMO: -6.63141 LUMO: -0.88981 factor:1 | -1 (1.10993) | -1 | -1 |
| G: -5683.64846 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11946.97302 HOMO: -6.92258 LUMO: -0.82178 factor:1 | -1 (1.04113) | -1 | -1 |
| G: -5683.64846 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11946.71903 HOMO: -6.55794 LUMO: -0.80818 factor:1 | -1 (1.29513) | -1 | -1 |
| G: -5683.64846 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.13516 HOMO: -6.95251 LUMO: -0.97145 factor:1 | 1 (-0.12101) | -1 | -1 |
| G: -5683.64846 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.73014 HOMO: -7.37701 LUMO: 0.14150 factor:1 | 1 (-0.71599) | -1 | -1 |
| G: -5683.64846 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.76989 HOMO: -6.74842 LUMO: -0.68028 factor:1 | 1 (-0.75574) | -1 | -1 |
| G: -5683.64846 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.83371 HOMO: -6.65046 LUMO: -0.52518 factor:1 | -1 (0.18044) | -1 | -1 |
| G: -5683.64846 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.92615 HOMO: -6.91441 LUMO: -1.13199 factor:1 | -1 (0.08800) | -1 | -1 |
| G: -5683.64846 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.90033 HOMO: -7.00965 LUMO: -1.00682 factor:1 | -1 (0.11383) | -1 | -1 |
| G: -5683.64846 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.68321 HOMO: -6.55794 LUMO: -0.54967 factor:1 | -1 (0.33094) | -1 | -1 |
| G: -5683.64846 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11946.95484 HOMO: -6.71577 LUMO: -0.53879 factor:1 | -1 (1.05931) | -1 | -1 |
| G: -5683.64846 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.32779 HOMO: -6.88992 LUMO: -0.55511 factor:1 | 1 (-0.31364) | -1 | -1 |
| G: -5683.64846 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.46201 HOMO: -6.74026 LUMO: -0.60681 factor:1 | -1 (0.55215) | -1 | -1 |
| G: -5683.64846 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.05128 HOMO: -6.76747 LUMO: -0.50885 factor:1 | 1 (-2.03713) | -1 | -1 |
| G: -5683.64846 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.24226 HOMO: -6.87904 LUMO: -0.92519 factor:1 | 1 (-1.22810) | -1 | -1 |
| G: -5683.64846 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.53007 HOMO: -6.53073 LUMO: -0.53062 factor:1 | 1 (-1.51592) | -1 | -1 |
| G: -5683.64846 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.04682 HOMO: -6.97700 LUMO: -0.98505 factor:1 | 1 (-2.03266) | -1 | -1 |
| G: -5683.64846 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.68077 HOMO: -6.96884 LUMO: -0.79185 factor:1 | 1 (-1.66662) | -1 | -1 |
| G: -5683.64846 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.88805 HOMO: -6.60420 LUMO: -0.31021 factor:1 | 1 (-0.87389) | -1 | -1 |
| G: -5683.64846 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.22669 HOMO: -6.68584 LUMO: -0.63947 factor:1 | 1 (-1.21254) | -1 | -1 |
| G: -5683.64846 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.85221 HOMO: -6.41917 LUMO: -0.35103 factor:1 | 1 (-0.83806) | -1 | -1 |
| G: -5683.64846 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.31269 HOMO: -6.73482 LUMO: -0.70477 factor:1 | 1 (-0.29854) | -1 | -1 |
| G: -5683.64846 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.57057 HOMO: -6.71305 LUMO: -0.85716 factor:1 | 1 (-0.55642) | -1 | -1 |
| G: -5683.64846 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.77412 HOMO: -6.70761 LUMO: -0.63403 factor:1 | -1 (0.24003) | -1 | -1 |
| G: -5683.64846 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.19429 HOMO: -6.37563 LUMO: -0.38640 factor:1 | 1 (-0.18014) | -1 | -1 |
| G: -5683.64846 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.96210 HOMO: -6.27495 LUMO: -0.54967 factor:1 | -1 (0.05206) | -1 | -1 |
| G: -5683.64846 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.76914 HOMO: -6.98516 LUMO: 0.38096 factor:1 | -1 (0.24501) | -1 | -1 |
| G: -5683.64846 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.83974 HOMO: -6.47087 LUMO: -0.40001 factor:1 | 1 (-1.82558) | -1 | -1 |
| G: -5683.64846 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.97949 HOMO: -6.59876 LUMO: 0.20681 factor:1 | 1 (-1.96534) | -1 | -1 |
| G: -5683.64846 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.31132 HOMO: -6.89809 LUMO: 0.14966 factor:1 | 1 (-1.29717) | -1 | -1 |
| G: -5683.64846 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.13608 HOMO: -6.76203 LUMO: 2.11432 factor:1 | 1 (-1.12193) | -1 | -1 |
| G: -5683.64846 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.05604 HOMO: -6.58516 LUMO: 1.75786 factor:1 | 1 (-2.04189) | -1 | -1 |
| G: -5683.64846 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.19624 HOMO: -6.37835 LUMO: 1.84493 factor:1 | 1 (-1.18209) | -1 | -1 |
| G: -5683.64846 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.75138 HOMO: -6.83550 LUMO: 1.74425 factor:1 | 1 (-1.73723) | -1 | -1 |
| G: -5683.64846 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.24285 HOMO: -6.65318 LUMO: 1.79051 factor:1 | 1 (-1.22870) | -1 | -1 |
| G: -5683.64846 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.81811 HOMO: -6.68584 LUMO: 2.11160 factor:1 | 1 (-0.80396) | -1 | -1 |
| G: -5683.64846 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.37204 HOMO: -6.36202 LUMO: 1.85037 factor:1 | 1 (-0.35788) | -1 | -1 |
| G: -5683.64846 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.80472 HOMO: -6.68312 LUMO: 2.23133 factor:1 | 1 (-0.79057) | -1 | -1 |
| G: -5683.64846 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.87751 HOMO: -6.66679 LUMO: 2.14154 factor:1 | 1 (-1.86335) | -1 | -1 |
| G: -5683.64846 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.13152 HOMO: -6.50896 LUMO: 1.92657 factor:1 | 1 (-2.11737) | -1 | -1 |
| G: -5683.64846 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.77537 HOMO: -6.63686 LUMO: 2.22317 factor:1 | 1 (-2.76122) | -1 | -1 |
| G: -5683.64846 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.70832 HOMO: -6.58788 LUMO: 2.17419 factor:1 | 1 (-2.69417) | -1 | -1 |
| G: -5683.64846 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.97090 HOMO: -6.72665 LUMO: 2.12249 factor:1 | 1 (-1.95674) | -1 | -1 |
| G: -5683.64846 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.94057 HOMO: -6.28311 LUMO: 1.91024 factor:1 | -1 (0.07358) | -1 | -1 |
| G: -5683.64846 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.96512 HOMO: -6.56067 LUMO: 2.27487 factor:1 | -1 (0.04903) | -1 | -1 |
| G: -5683.64846 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.19527 HOMO: -6.83006 LUMO: 2.28031 factor:1 | 1 (-0.18112) | -1 | -1 |
| G: -5683.64846 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.96837 HOMO: -6.45182 LUMO: 1.62724 factor:1 | 1 (-0.95422) | -1 | -1 |
| G: -5683.64846 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.29908 HOMO: -6.78380 LUMO: 1.83677 factor:1 | 1 (-0.28493) | -1 | -1 |
| G: -5683.64846 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.85564 HOMO: -6.23413 LUMO: 1.80956 factor:1 | 1 (-0.84148) | -1 | -1 |
| G: -5683.64846 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.80053 HOMO: -6.74298 LUMO: 2.16875 factor:1 | 1 (-0.78638) | -1 | -1 |
| G: -5683.64846 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.18664 HOMO: -6.81645 LUMO: 2.50073 factor:1 | 1 (-0.17249) | -1 | -1 |
| G: -5683.64846 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.19777 HOMO: -6.71033 LUMO: 1.96466 factor:1 | 1 (-0.18362) | -1 | -1 |
| G: -5683.64846 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.98261 HOMO: -6.83550 LUMO: 2.04358 factor:1 | 1 (-0.96845) | -1 | -1 |
| G: -5683.64846 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.28520 HOMO: -6.60965 LUMO: 2.38100 factor:1 | 1 (-0.27105) | -1 | -1 |
| G: -5683.64846 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.02127 HOMO: -6.73210 LUMO: 2.26127 factor:1 | 1 (-1.00712) | -1 | -1 |
| G: -5683.64846 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.43604 HOMO: -6.76203 LUMO: 2.13609 factor:1 | 1 (-0.42189) | -1 | -1 |
| G: -5683.64846 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.67005 HOMO: -6.71033 LUMO: 2.05990 factor:1 | 1 (-1.65589) | -1 | -1 |
| G: -5683.64846 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.62812 HOMO: -6.50896 LUMO: 2.32385 factor:1 | 1 (-0.61397) | -1 | -1 |
| G: -5683.64846 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.64668 HOMO: -6.53345 LUMO: 1.74425 factor:1 | 1 (-0.63253) | -1 | -1 |
| G: -5683.64846 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.79893 HOMO: -6.25862 LUMO: 1.63540 factor:1 | 1 (-0.78478) | -1 | -1 |
| G: -5683.64846 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.63634 HOMO: -5.90759 LUMO: 1.78779 factor:1 | 1 (-0.62219) | -1 | -1 |
| G: -5683.64846 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.73299 HOMO: -6.09807 LUMO: 1.99732 factor:1 | 1 (-0.71884) | -1 | -1 |
| G: -5683.64846 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.75307 HOMO: -5.92392 LUMO: 1.99732 factor:1 | 1 (-1.73892) | -1 | -1 |
| G: -5683.64846 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.61886 HOMO: -6.45182 LUMO: 1.72248 factor:1 | 1 (-1.60471) | -1 | -1 |
| G: -5683.64846 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.42932 HOMO: -6.53073 LUMO: 1.82588 factor:1 | 1 (-0.41516) | -1 | -1 |
| G: -5683.64846 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.46670 HOMO: -6.40828 LUMO: 2.05174 factor:1 | 1 (-0.45255) | -1 | -1 |
| G: -5683.64846 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.76803 HOMO: -6.60420 LUMO: -0.82450 factor:1 | 1 (-2.75387) | -1 | -1 |
| G: -5683.64846 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.01207 HOMO: -6.76747 LUMO: -0.57144 factor:1 | 1 (-1.99791) | -1 | -1 |
| G: -5683.64846 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.85032 HOMO: -6.67767 LUMO: -0.59321 factor:1 | 1 (-1.83617) | -1 | -1 |
| G: -5683.64846 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.78020 HOMO: -6.65863 LUMO: -0.57416 factor:1 | 1 (-1.76605) | -1 | -1 |
| G: -5683.64846 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.77674 HOMO: -6.49808 LUMO: -0.54695 factor:1 | 1 (-1.76259) | -1 | -1 |
| G: -5683.64846 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.51282 HOMO: -6.50080 LUMO: -0.61498 factor:1 | 1 (-1.49867) | -1 | -1 |
| G: -5683.64846 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.29630 HOMO: -6.74842 LUMO: -0.51974 factor:1 | 1 (-1.28215) | -1 | -1 |
| G: -5683.64846 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.41869 HOMO: -6.13345 LUMO: 0.67756 factor:1 | 1 (-1.40454) | -1 | -1 |
| G: -5683.64846 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.57143 HOMO: -6.48719 LUMO: 0.52790 factor:1 | 1 (-1.55728) | -1 | -1 |
| G: -5683.64846 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.47641 HOMO: -6.35930 LUMO: 0.74015 factor:1 | 1 (-1.46226) | -1 | -1 |
| G: -5683.64846 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.50615 HOMO: -6.41644 LUMO: 0.22313 factor:1 | 1 (-1.49200) | -1 | -1 |
| G: -5683.64846 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.54938 HOMO: -6.85727 LUMO: -0.00272 factor:1 | -1 (0.46477) | -1 | -1 |
| G: -5683.64846 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11946.62221 HOMO: -6.84638 LUMO: 0.24762 factor:1 | -1 (1.39194) | -1 | -1 |
| G: -5683.64846 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.39713 HOMO: -6.66951 LUMO: 0.39184 factor:1 | -1 (0.61702) | -1 | -1 |
| G: -5683.64846 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.98581 HOMO: -6.62597 LUMO: -0.65035 factor:1 | 1 (-1.97166) | -1 | -1 |
| G: -5683.64846 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.30797 HOMO: -7.13755 LUMO: 0.45715 factor:1 | 1 (-1.29382) | -1 | -1 |
| G: -5683.64846 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.83329 HOMO: -7.12666 LUMO: 0.45171 factor:1 | 1 (-1.81914) | -1 | -1 |
| G: -5683.64846 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.33711 HOMO: -6.46270 LUMO: -0.46259 factor:1 | 1 (-1.32296) | -1 | -1 |
| G: -5683.64846 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.87522 HOMO: -6.36202 LUMO: -0.29660 factor:1 | 1 (-1.86107) | -1 | -1 |
| G: -5683.64846 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.67116 HOMO: -6.28583 LUMO: 0.40545 factor:1 | 1 (-1.65701) | -1 | -1 |
| G: -5683.64846 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.15670 HOMO: -6.70761 LUMO: 0.41906 factor:1 | 1 (-1.14255) | -1 | -1 |
| G: -5683.64846 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.59048 HOMO: -6.76203 LUMO: -0.60954 factor:1 | 1 (-1.57633) | -1 | -1 |
| G: -5683.64846 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.28244 HOMO: -6.85999 LUMO: -0.75103 factor:1 | -1 (0.73171) | -1 | -1 |
| G: -5683.64846 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11946.62237 HOMO: -7.19741 LUMO: -1.00954 factor:1 | -1 (1.39178) | -1 | -1 |
| G: -5683.64846 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.40811 HOMO: -6.58243 LUMO: -0.33470 factor:1 | 1 (-1.39396) | -1 | -1 |
| G: -5683.64846 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.02375 HOMO: -7.22190 LUMO: 0.49253 factor:1 | 1 (-1.00960) | -1 | -1 |
| G: -5683.64846 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.76262 HOMO: -7.22462 LUMO: 0.51974 factor:1 | 1 (-1.74847) | -1 | -1 |
| G: -5683.64846 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.10538 HOMO: -7.08584 LUMO: -0.68301 factor:1 | 1 (-1.09123) | -1 | -1 |
| G: -5683.64846 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.88608 HOMO: -6.68584 LUMO: -0.29660 factor:1 | 1 (-1.87193) | -1 | -1 |
| G: -5683.64846 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.14168 HOMO: -6.33753 LUMO: -0.48436 factor:1 | 1 (-1.12753) | -1 | -1 |
| G: -5683.64846 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.12180 HOMO: -7.15932 LUMO: 0.55511 factor:1 | 1 (-0.10765) | -1 | -1 |
| G: -5683.64846 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.05011 HOMO: -6.57427 LUMO: 2.01908 factor:1 | -1 (0.96404) | -1 | -1 |
| G: -5683.64846 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.00107 HOMO: -6.75659 LUMO: 2.22045 factor:1 | -1 (1.01308) | -1 | -1 |
| G: -5683.64846 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.42481 HOMO: -6.73482 LUMO: 2.20956 factor:1 | -1 (0.58934) | -1 | -1 |
| G: -5683.64846 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11946.09686 HOMO: -6.74026 LUMO: 1.76602 factor:1 | -1 (1.91729) | -1 | -1 |
| G: -5683.64846 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11945.95471 HOMO: -6.95523 LUMO: 1.94834 factor:1 | -1 (2.05944) | -1 | -1 |
| G: -5683.64846 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.11225 HOMO: -6.33209 LUMO: 1.87486 factor:1 | 1 (-0.09810) | -1 | -1 |
| G: -5683.64846 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.07598 HOMO: -6.71033 LUMO: 2.12521 factor:1 | -1 (0.93817) | -1 | -1 |
| G: -5683.64846 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.31606 HOMO: -6.50080 LUMO: 2.04902 factor:1 | 1 (-0.30191) | -1 | -1 |
| G: -5683.64846 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.53722 HOMO: -6.76475 LUMO: 1.94017 factor:1 | -1 (0.47693) | -1 | -1 |
| G: -5683.64846 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11946.97626 HOMO: -6.53073 LUMO: 2.08983 factor:1 | -1 (1.03790) | -1 | -1 |
| G: -5683.64846 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.70105 HOMO: -6.69944 LUMO: 2.20684 factor:1 | 1 (-0.68690) | -1 | -1 |
| G: -5683.64846 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.15797 HOMO: -6.34570 LUMO: 1.80684 factor:1 | 1 (-2.14382) | -1 | -1 |
| G: -5683.64846 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.25986 HOMO: -6.78380 LUMO: 1.95922 factor:1 | 1 (-1.24571) | -1 | -1 |
| G: -5683.64846 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.11999 HOMO: -6.93618 LUMO: 1.76058 factor:1 | 1 (-2.10583) | -1 | -1 |
| G: -5683.64846 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.24500 HOMO: -6.93346 LUMO: 1.79595 factor:1 | 1 (-1.23085) | -1 | -1 |
| G: -5683.64846 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.87353 HOMO: -6.29671 LUMO: 1.75241 factor:1 | 1 (-1.85938) | -1 | -1 |
| G: -5683.64846 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.14925 HOMO: -6.77019 LUMO: 1.74697 factor:1 | 1 (-1.13510) | -1 | -1 |
| G: -5683.64846 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.74113 HOMO: -6.87360 LUMO: 1.91024 factor:1 | 1 (-0.72698) | -1 | -1 |
| G: -5683.64846 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.50378 HOMO: -6.32665 LUMO: 1.87759 factor:1 | -1 (0.51038) | -1 | -1 |
| G: -5683.64846 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.17909 HOMO: -6.99877 LUMO: 1.99187 factor:1 | -1 (0.83506) | -1 | -1 |
| G: -5683.64846 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.12806 HOMO: -6.72665 LUMO: 2.12521 factor:1 | 1 (-0.11391) | -1 | -1 |
| G: -5683.64846 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.85419 HOMO: -6.67767 LUMO: 2.43814 factor:1 | 1 (-0.84004) | -1 | -1 |
| G: -5683.64846 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.79560 HOMO: -6.99605 LUMO: 1.79051 factor:1 | 1 (-1.78145) | -1 | -1 |
| G: -5683.64846 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.02500 HOMO: -6.25046 LUMO: 1.77146 factor:1 | 1 (-1.01085) | -1 | -1 |
| G: -5683.64846 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.56575 HOMO: -6.30488 LUMO: 1.90480 factor:1 | 1 (-1.55159) | -1 | -1 |
| G: -5683.64846 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.07699 HOMO: -6.38379 LUMO: 1.68438 factor:1 | 1 (-2.06284) | -1 | -1 |
| G: -5683.64846 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.28778 HOMO: -6.78924 LUMO: 2.01364 factor:1 | 1 (-1.27363) | -1 | -1 |
| G: -5683.64846 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.12133 HOMO: -6.15249 LUMO: 1.98643 factor:1 | 1 (-1.10718) | -1 | -1 |
| G: -5683.64846 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.94146 HOMO: -6.19331 LUMO: 2.14154 factor:1 | 1 (-0.92731) | -1 | -1 |
| G: -5683.64846 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.21196 HOMO: -6.05998 LUMO: 2.12521 factor:1 | -1 (0.80219) | -1 | -1 |
| G: -5683.64846 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.05535 HOMO: -6.67223 LUMO: 1.91840 factor:1 | 1 (-0.04120) | -1 | -1 |
| G: -5683.64846 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.37059 HOMO: -6.79196 LUMO: 2.18507 factor:1 | 1 (-0.35644) | -1 | -1 |
| G: -5683.64846 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.52908 HOMO: -6.93346 LUMO: 1.78235 factor:1 | -1 (0.48507) | -1 | -1 |
| G: -5683.64846 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.70211 HOMO: -6.16882 LUMO: 1.80956 factor:1 | 1 (-0.68796) | -1 | -1 |
| G: -5683.64846 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.95454 HOMO: -6.72665 LUMO: 2.07895 factor:1 | 1 (-1.94039) | -1 | -1 |
| G: -5683.64846 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.31608 HOMO: -6.73210 LUMO: 1.97827 factor:1 | 1 (-1.30193) | -1 | -1 |
| G: -5683.64846 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.10555 HOMO: -6.84638 LUMO: 1.87214 factor:1 | 1 (-1.09139) | -1 | -1 |
| G: -5683.64846 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.00458 HOMO: -6.83006 LUMO: 2.36195 factor:1 | 1 (-1.99043) | -1 | -1 |
| G: -5683.64846 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.96417 HOMO: -6.97700 LUMO: 1.91024 factor:1 | 1 (-1.95002) | -1 | -1 |
| G: -5683.64846 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.24672 HOMO: -6.20420 LUMO: 1.81772 factor:1 | 1 (-1.23257) | -1 | -1 |
| G: -5683.64846 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.10023 HOMO: -7.09129 LUMO: 2.10344 factor:1 | 1 (-2.08608) | 1 | 1 |
| G: -5683.64846 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.40852 HOMO: -6.77564 LUMO: 2.14970 factor:1 | 1 (-1.39437) | -1 | -1 |
| G: -5683.64846 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.80534 HOMO: -6.81645 LUMO: 1.85854 factor:1 | 1 (-1.79119) | -1 | -1 |
| G: -5683.64846 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.85679 HOMO: -6.50896 LUMO: 2.04358 factor:1 | -1 (0.15736) | -1 | -1 |
| G: -5683.64846 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.63618 HOMO: -6.89264 LUMO: 1.66262 factor:1 | 1 (-0.62203) | -1 | -1 |
| G: -5683.64846 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.04581 HOMO: -6.75931 LUMO: 2.23950 factor:1 | -1 (0.96834) | -1 | -1 |
| G: -5683.64846 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.68454 HOMO: -6.50080 LUMO: 1.67622 factor:1 | -1 (0.32961) | -1 | -1 |
| G: -5683.64846 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.93766 HOMO: -6.30216 LUMO: 2.24222 factor:1 | -1 (0.07649) | -1 | -1 |
| G: -5683.64846 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.89528 HOMO: -7.18108 LUMO: 2.10072 factor:1 | 1 (-0.88113) | 1 | 1 |
| G: -5683.64846 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.46623 HOMO: -6.54162 LUMO: 2.35378 factor:1 | 1 (-1.45208) | -1 | -1 |
| G: -5683.64846 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.32674 HOMO: -5.98650 LUMO: 1.48302 factor:1 | 1 (-2.31259) | -1 | -1 |
| G: -5683.64846 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.24119 HOMO: -7.15115 LUMO: 2.14970 factor:1 | 1 (-1.22704) | 1 | 1 |
| G: -5683.64846 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.94279 HOMO: -6.45454 LUMO: 2.15786 factor:1 | 1 (-1.92863) | -1 | -1 |
| G: -5683.64846 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.91964 HOMO: -7.06952 LUMO: 2.14970 factor:1 | 1 (-0.90549) | 1 | 1 |
| G: -5683.64846 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11946.76441 HOMO: -6.93618 LUMO: 1.86942 factor:1 | -1 (1.24974) | -1 | -1 |
| G: -5683.64846 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.58774 HOMO: -6.63141 LUMO: 1.92657 factor:1 | 1 (-0.57359) | -1 | -1 |
| G: -5683.64846 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.71417 HOMO: -6.51441 LUMO: -0.44355 factor:1 | -1 (0.29998) | -1 | -1 |
| G: -5683.64846 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.77253 HOMO: -6.82734 LUMO: -1.03131 factor:1 | 1 (-0.75838) | -1 | -1 |
| G: -5683.64846 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.86016 HOMO: -6.58788 LUMO: -0.82995 factor:1 | -1 (0.15399) | -1 | -1 |
| G: -5683.64846 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.87863 HOMO: -6.43277 LUMO: -0.40817 factor:1 | 1 (-0.86448) | -1 | -1 |
| G: -5683.64846 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.63035 HOMO: -6.78924 LUMO: -0.72110 factor:1 | 1 (-0.61620) | -1 | -1 |
| G: -5683.64846 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.34866 HOMO: -7.28177 LUMO: 0.36735 factor:1 | 1 (-0.33451) | -1 | -1 |
| G: -5683.64846 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.07654 HOMO: -6.47903 LUMO: -0.46259 factor:1 | 1 (-1.06239) | -1 | -1 |
| G: -5683.64846 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.98975 HOMO: -6.67495 LUMO: -0.75376 factor:1 | 1 (-1.97560) | -1 | -1 |
| G: -5683.64846 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.07967 HOMO: -6.71033 LUMO: -0.71838 factor:1 | 1 (-1.06552) | -1 | -1 |
| G: -5683.64846 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.50871 HOMO: -6.79740 LUMO: -0.79185 factor:1 | 1 (-1.49456) | -1 | -1 |
| G: -5683.64846 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.01088 HOMO: -6.08719 LUMO: -0.63675 factor:1 | 1 (-0.99673) | -1 | -1 |
| G: -5683.64846 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.51938 HOMO: -6.84094 LUMO: 0.42994 factor:1 | 1 (-1.50523) | -1 | -1 |
| G: -5683.64846 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.02111 HOMO: -6.59604 LUMO: 0.25851 factor:1 | 1 (-1.00696) | -1 | -1 |
| G: -5683.64846 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.76791 HOMO: -6.82462 LUMO: 0.08708 factor:1 | 1 (-0.75376) | -1 | -1 |
| G: -5683.64846 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.99224 HOMO: -6.54706 LUMO: 0.44082 factor:1 | 1 (-0.97809) | -1 | -1 |
| G: -5683.64846 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.89732 HOMO: -6.99333 LUMO: 0.32109 factor:1 | 1 (-0.88317) | -1 | -1 |
| G: -5683.64846 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.85446 HOMO: -6.29944 LUMO: -0.57144 factor:1 | 1 (-1.84031) | -1 | -1 |
| G: -5683.64846 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.26880 HOMO: -6.57699 LUMO: -0.46531 factor:1 | 1 (-0.25464) | -1 | -1 |
| G: -5683.64846 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.13619 HOMO: -6.24773 LUMO: -0.53879 factor:1 | 1 (-0.12204) | -1 | -1 |
| G: -5683.64846 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.79362 HOMO: -6.96067 LUMO: -0.67212 factor:1 | 1 (-0.77947) | -1 | -1 |
| G: -5683.64846 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.66937 HOMO: -7.24095 LUMO: -0.09252 factor:1 | 1 (-0.65522) | -1 | -1 |
| G: -5683.64846 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.40797 HOMO: -6.33481 LUMO: -0.46531 factor:1 | 1 (-1.39382) | -1 | -1 |
| G: -5683.64846 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.92535 HOMO: -6.43549 LUMO: -0.33198 factor:1 | 1 (-0.91120) | -1 | -1 |
| G: -5683.64846 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.94120 HOMO: -6.53073 LUMO: 0.44899 factor:1 | -1 (0.07295) | -1 | -1 |
| G: -5683.64846 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.64342 HOMO: -6.69128 LUMO: 0.47620 factor:1 | 1 (-0.62926) | -1 | -1 |
| G: -5683.64846 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.75000 HOMO: -6.65318 LUMO: 0.52246 factor:1 | 1 (-0.73585) | -1 | -1 |
| G: -5683.64846 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.89687 HOMO: -6.71305 LUMO: 0.41089 factor:1 | -1 (0.11728) | -1 | -1 |
| G: -5683.64846 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.55341 HOMO: -6.70216 LUMO: 0.19864 factor:1 | -1 (0.46074) | -1 | -1 |
| G: -5683.64846 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11946.34579 HOMO: -6.41100 LUMO: 0.34558 factor:1 | -1 (1.66836) | -1 | -1 |
| G: -5683.64846 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11946.71854 HOMO: -7.01237 LUMO: 0.02993 factor:1 | -1 (1.29562) | -1 | -1 |
| G: -5683.64846 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11946.74670 HOMO: -6.85999 LUMO: 0.18776 factor:1 | -1 (1.26745) | -1 | -1 |
| G: -5683.64846 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11946.73350 HOMO: -6.62869 LUMO: 0.48708 factor:1 | -1 (1.28065) | -1 | -1 |
| G: -5683.64846 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.01037 HOMO: -6.43821 LUMO: -0.45715 factor:1 | -1 (0.00378) | -1 | -1 |
| G: -5683.64846 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.99812 HOMO: -6.43277 LUMO: -0.72110 factor:1 | -1 (0.01603) | -1 | -1 |
| G: -5683.64846 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.60753 HOMO: -7.10761 LUMO: 0.43266 factor:1 | -1 (0.40662) | -1 | -1 |
| G: -5683.64846 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.64211 HOMO: -6.57699 LUMO: -0.61498 factor:1 | 1 (-0.62796) | -1 | -1 |
| G: -5683.64846 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.54208 HOMO: -6.82189 LUMO: -0.75648 factor:1 | 1 (-0.52793) | -1 | -1 |
| G: -5683.64846 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.48716 HOMO: -6.55794 LUMO: -0.67212 factor:1 | 1 (-1.47301) | -1 | -1 |
| G: -5683.64846 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.05653 HOMO: -6.69128 LUMO: 1.88575 factor:1 | 1 (-2.04238) | -1 | -1 |
| G: -5683.64846 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.65942 HOMO: -6.65591 LUMO: 1.70888 factor:1 | 1 (-0.64526) | -1 | -1 |
| G: -5683.64846 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.04778 HOMO: -6.58788 LUMO: 1.68438 factor:1 | 1 (-1.03362) | -1 | -1 |
| G: -5683.64846 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.30288 HOMO: -6.46270 LUMO: 1.72520 factor:1 | 1 (-1.28873) | -1 | -1 |
| G: -5683.64846 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.02997 HOMO: -6.57427 LUMO: 1.73881 factor:1 | 1 (-2.01582) | -1 | -1 |
| G: -5683.64846 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.39222 HOMO: -6.45182 LUMO: 1.75241 factor:1 | 1 (-1.37807) | -1 | -1 |
| G: -5683.64846 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.00834 HOMO: -6.51441 LUMO: 1.78779 factor:1 | 1 (-1.99419) | -1 | -1 |
| G: -5683.64846 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.06810 HOMO: -6.67495 LUMO: 2.11705 factor:1 | 1 (-1.05395) | -1 | -1 |
| G: -5683.64846 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.63905 HOMO: -6.22597 LUMO: 1.96466 factor:1 | 1 (-1.62490) | -1 | -1 |
| G: -5683.64846 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.00933 HOMO: -6.68040 LUMO: 2.30753 factor:1 | 1 (-0.99517) | -1 | -1 |
| G: -5683.64846 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.69410 HOMO: -6.65046 LUMO: 2.18235 factor:1 | 1 (-1.67995) | -1 | -1 |
| G: -5683.64846 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.78708 HOMO: -6.38651 LUMO: 1.76874 factor:1 | 1 (-1.77293) | -1 | -1 |
| G: -5683.64846 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.96470 HOMO: -6.41644 LUMO: 2.09256 factor:1 | 1 (-0.95055) | -1 | -1 |
| G: -5683.64846 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.64741 HOMO: -6.14977 LUMO: 2.28031 factor:1 | 1 (-1.63325) | -1 | -1 |
| G: -5683.64846 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.47671 HOMO: -6.70489 LUMO: 2.43814 factor:1 | 1 (-1.46256) | -1 | -1 |
| G: -5683.64846 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.79877 HOMO: -6.78924 LUMO: 2.27215 factor:1 | -1 (0.21538) | -1 | -1 |
| G: -5683.64846 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.93026 HOMO: -6.86271 LUMO: 2.31025 factor:1 | -1 (0.08389) | -1 | -1 |
| G: -5683.64846 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.15568 HOMO: -6.51168 LUMO: 2.04630 factor:1 | 1 (-0.14153) | -1 | -1 |
| G: -5683.64846 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11946.68311 HOMO: -6.72665 LUMO: 2.13337 factor:1 | -1 (1.33104) | -1 | -1 |
| G: -5683.64846 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11946.64243 HOMO: -6.45998 LUMO: 2.16058 factor:1 | -1 (1.37173) | -1 | -1 |
| G: -5683.64846 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.47498 HOMO: -6.83822 LUMO: 2.20684 factor:1 | 1 (-0.46082) | -1 | -1 |
| G: -5683.64846 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.41756 HOMO: -6.68856 LUMO: 2.19324 factor:1 | 1 (-0.40341) | -1 | -1 |
| G: -5683.64846 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.93248 HOMO: -6.71577 LUMO: 2.16058 factor:1 | 1 (-0.91833) | -1 | -1 |
| G: -5683.64846 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.94384 HOMO: -6.82462 LUMO: 1.90208 factor:1 | -1 (0.07031) | -1 | -1 |
| G: -5683.64846 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.87702 HOMO: -6.61509 LUMO: 2.23950 factor:1 | 1 (-0.86287) | -1 | -1 |
| G: -5683.64846 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.97616 HOMO: -6.73754 LUMO: 1.84221 factor:1 | -1 (0.03799) | -1 | -1 |
| G: -5683.64846 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.57707 HOMO: -6.56611 LUMO: 1.94561 factor:1 | 1 (-0.56292) | -1 | -1 |
| G: -5683.64846 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.52164 HOMO: -6.67767 LUMO: 1.51840 factor:1 | 1 (-0.50749) | -1 | -1 |
| G: -5683.64846 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.48638 HOMO: -6.35658 LUMO: 2.16603 factor:1 | 1 (-0.47223) | -1 | -1 |
| G: -5683.64846 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.07355 HOMO: -6.35114 LUMO: 2.08983 factor:1 | 1 (-1.05939) | -1 | -1 |
| G: -5683.64846 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.01174 HOMO: -6.35114 LUMO: 2.10616 factor:1 | 1 (-1.99759) | -1 | -1 |
| G: -5683.64846 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.63151 HOMO: -6.71305 LUMO: 2.01636 factor:1 | 1 (-1.61736) | -1 | -1 |
| G: -5683.64846 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.06491 HOMO: -6.24773 LUMO: 1.98915 factor:1 | 1 (-2.05076) | -1 | -1 |
| G: -5683.64846 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.13110 HOMO: -6.53617 LUMO: 2.42726 factor:1 | 1 (-1.11695) | -1 | -1 |
| G: -5683.64846 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.09898 HOMO: -6.59332 LUMO: 1.82316 factor:1 | 1 (-2.08483) | -1 | -1 |
| G: -5683.64846 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.41616 HOMO: -6.41372 LUMO: 1.77418 factor:1 | 1 (-1.40201) | -1 | -1 |
| G: -5683.64846 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.65620 HOMO: -6.40284 LUMO: 1.88575 factor:1 | 1 (-0.64205) | -1 | -1 |
| G: -5683.64846 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.55657 HOMO: -6.11168 LUMO: 1.70888 factor:1 | 1 (-1.54242) | -1 | -1 |
| G: -5683.64846 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.67927 HOMO: -6.44910 LUMO: 2.23405 factor:1 | 1 (-1.66512) | -1 | -1 |
| G: -5683.64846 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.04408 HOMO: -6.24773 LUMO: 2.12793 factor:1 | 1 (-1.02992) | -1 | -1 |
| G: -5683.64846 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.90380 HOMO: -6.07358 LUMO: 1.89663 factor:1 | 1 (-0.88965) | -1 | -1 |
| G: -5683.64846 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.56032 HOMO: -6.66679 LUMO: 1.96738 factor:1 | -1 (0.45383) | -1 | -1 |
| G: -5683.64846 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.53365 HOMO: -6.68312 LUMO: 1.78235 factor:1 | -1 (0.48050) | -1 | -1 |
| G: -5683.64846 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.68050 HOMO: -6.70761 LUMO: 1.97555 factor:1 | 1 (-0.66635) | -1 | -1 |
| G: -5683.64846 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.80521 HOMO: -6.15794 LUMO: 2.00548 factor:1 | 1 (-0.79106) | -1 | -1 |
| G: -5683.64846 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.57931 HOMO: -6.52257 LUMO: 1.96738 factor:1 | 1 (-0.56515) | -1 | -1 |
| G: -5683.64846 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.53422 HOMO: -6.25590 LUMO: 1.86670 factor:1 | 1 (-0.52006) | -1 | -1 |
| G: -5683.64846 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.97624 HOMO: -6.30216 LUMO: 1.84765 factor:1 | 1 (-0.96209) | -1 | -1 |
| G: -5683.64846 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.33091 HOMO: -6.76747 LUMO: 2.20956 factor:1 | 1 (-1.31676) | -1 | -1 |
| G: -5683.64846 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.51285 HOMO: -6.14161 LUMO: 1.80684 factor:1 | 1 (-1.49869) | -1 | -1 |
| G: -5683.64846 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.84829 HOMO: -6.81373 LUMO: 1.91024 factor:1 | 1 (-0.83414) | -1 | -1 |
| G: -5683.64846 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.83272 HOMO: -6.81917 LUMO: 2.34834 factor:1 | 1 (-1.81856) | -1 | -1 |
| G: -5683.64846 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.08710 HOMO: -6.72121 LUMO: 1.90208 factor:1 | 1 (-1.07294) | -1 | -1 |
| G: -5683.64846 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.05521 HOMO: -7.51851 LUMO: 0.26939 factor:1 | 1 (-1.04105) | -1 | -1 |
| G: -5683.64846 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.52166 HOMO: -6.65318 LUMO: -0.57144 factor:1 | 1 (-1.50751) | -1 | -1 |
| G: -5683.64846 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.97759 HOMO: -6.77564 LUMO: -0.72654 factor:1 | 1 (-1.96344) | -1 | -1 |
| G: -5683.64846 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.06546 HOMO: -6.80557 LUMO: -0.60954 factor:1 | 1 (-1.05131) | -1 | -1 |
| G: -5683.64846 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.03463 HOMO: -7.35524 LUMO: 0.27483 factor:1 | 1 (-1.02048) | -1 | -1 |
| G: -5683.64846 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.05627 HOMO: -6.94979 LUMO: -0.83811 factor:1 | 1 (-1.04211) | -1 | -1 |
| G: -5683.64846 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.48249 HOMO: -6.13345 LUMO: -0.67212 factor:1 | 1 (-0.46834) | -1 | -1 |
| G: -5683.64846 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11946.53059 HOMO: -6.47359 LUMO: -0.59321 factor:1 | -1 (1.48356) | -1 | -1 |
| G: -5683.64846 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11946.88559 HOMO: -6.52257 LUMO: -0.54695 factor:1 | -1 (1.12857) | -1 | -1 |
| G: -5683.64846 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.39644 HOMO: -6.61781 LUMO: -0.69661 factor:1 | 1 (-0.38229) | -1 | -1 |
| G: -5683.64846 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.21354 HOMO: -6.77564 LUMO: -0.80001 factor:1 | -1 (0.80061) | -1 | -1 |
| G: -5683.64846 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.45411 HOMO: -7.35252 LUMO: -1.00410 factor:1 | -1 (0.56004) | -1 | -1 |
| G: -5683.64846 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.17237 HOMO: -6.35386 LUMO: -0.38912 factor:1 | -1 (0.84178) | -1 | -1 |
| G: -5683.64846 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.17849 HOMO: -6.80285 LUMO: -0.52246 factor:1 | -1 (0.83566) | -1 | -1 |
| G: -5683.64846 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11946.90591 HOMO: -7.23279 LUMO: 0.30477 factor:1 | -1 (1.10824) | -1 | -1 |
| G: -5683.64846 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.08023 HOMO: -7.13483 LUMO: -0.76192 factor:1 | -1 (0.93392) | -1 | -1 |
| G: -5683.64846 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.51586 HOMO: -6.71849 LUMO: -0.48164 factor:1 | -1 (0.49829) | -1 | -1 |
| G: -5683.64846 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11946.72387 HOMO: -6.85455 LUMO: -0.69389 factor:1 | -1 (1.29028) | -1 | -1 |
| G: -5683.64846 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11946.76243 HOMO: -6.96339 LUMO: -0.73743 factor:1 | -1 (1.25172) | -1 | -1 |
| G: -5683.64846 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.07584 HOMO: -7.50490 LUMO: 0.28844 factor:1 | 1 (-0.06169) | -1 | -1 |
| G: -5683.64846 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.37465 HOMO: -6.63958 LUMO: -0.50069 factor:1 | 1 (-0.36050) | -1 | -1 |
| G: -5683.64846 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.29691 HOMO: -6.78924 LUMO: -0.69661 factor:1 | 1 (-0.28275) | -1 | -1 |
| G: -5683.64846 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.11690 HOMO: -7.44776 LUMO: 0.33742 factor:1 | 1 (-0.10275) | -1 | -1 |
| G: -5683.64846 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.81067 HOMO: -6.15249 LUMO: 0.66396 factor:1 | -1 (0.20349) | -1 | -1 |
| G: -5683.64846 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.51297 HOMO: -6.17426 LUMO: 0.55511 factor:1 | -1 (0.50118) | -1 | -1 |
| G: -5683.64846 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.38083 HOMO: -6.83550 LUMO: 0.28844 factor:1 | -1 (0.63332) | -1 | -1 |
| G: -5683.64846 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.67420 HOMO: -6.32393 LUMO: 0.47620 factor:1 | -1 (0.33995) | -1 | -1 |
| G: -5683.64846 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.16181 HOMO: -6.32937 LUMO: 0.45987 factor:1 | -1 (0.85234) | -1 | -1 |
| G: -5683.64846 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.92668 HOMO: -7.37429 LUMO: 0.09252 factor:1 | 1 (-1.91253) | -1 | -1 |
| G: -5683.64846 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.99005 HOMO: -6.54434 LUMO: -0.39729 factor:1 | 1 (-1.97590) | -1 | -1 |
| G: -5683.64846 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.26184 HOMO: -7.35524 LUMO: 0.28028 factor:1 | 1 (-2.24769) | -1 | -1 |
| G: -5683.64846 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.57500 HOMO: -6.95523 LUMO: -0.86804 factor:1 | 1 (-1.56085) | -1 | -1 |
| G: -5683.64846 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.08820 HOMO: -6.63958 LUMO: -0.65307 factor:1 | 1 (-2.07405) | -1 | -1 |
| G: -5683.64846 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.23220 HOMO: -6.73482 LUMO: -0.67212 factor:1 | 1 (-0.21804) | -1 | -1 |
| G: -5683.64846 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.30270 HOMO: -6.37835 LUMO: -0.53606 factor:1 | 1 (-0.28855) | -1 | -1 |
| G: -5683.64846 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.08003 HOMO: -6.71849 LUMO: -0.61226 factor:1 | 1 (-0.06588) | -1 | -1 |
| G: -5683.64846 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.84643 HOMO: -6.68584 LUMO: -1.11022 factor:1 | 1 (-1.83228) | -1 | -1 |
| G: -5683.64846 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.72354 HOMO: -6.80285 LUMO: -0.79185 factor:1 | 1 (-1.70939) | -1 | -1 |
| G: -5683.64846 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.12628 HOMO: -7.14571 LUMO: -0.94696 factor:1 | 1 (-1.11213) | -1 | -1 |
| G: -5683.64846 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.05893 HOMO: -7.16204 LUMO: -0.66124 factor:1 | 1 (-1.04478) | -1 | -1 |
| G: -5683.64846 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.32876 HOMO: -6.54978 LUMO: -0.54967 factor:1 | 1 (-1.31461) | -1 | -1 |
| G: -5683.64846 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.12227 HOMO: -6.75114 LUMO: -0.70750 factor:1 | 1 (-2.10812) | -1 | -1 |
| G: -5683.64846 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.18875 HOMO: -7.22190 LUMO: 0.39184 factor:1 | 1 (-2.17460) | -1 | -1 |
| G: -5683.64846 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.60158 HOMO: -7.43959 LUMO: 0.30477 factor:1 | 1 (-1.58743) | -1 | -1 |
| G: -5683.64846 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.93889 HOMO: -6.87360 LUMO: -0.77552 factor:1 | 1 (-1.92474) | -1 | -1 |
| G: -5683.64846 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.78180 HOMO: -6.82734 LUMO: -0.59593 factor:1 | 1 (-1.76765) | -1 | -1 |
| G: -5683.64846 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.45382 HOMO: -6.65318 LUMO: -0.46259 factor:1 | 1 (-2.43966) | -1 | -1 |
| G: -5683.64846 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.87459 HOMO: -7.05863 LUMO: -1.17009 factor:1 | 1 (-1.86044) | -1 | -1 |
| G: -5683.64846 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.35537 HOMO: -6.57427 LUMO: -0.48708 factor:1 | 1 (-1.34122) | -1 | -1 |
| G: -5683.64846 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.51102 HOMO: -6.60420 LUMO: -0.38096 factor:1 | 1 (-1.49687) | -1 | -1 |
| G: -5683.64846 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.86394 HOMO: -6.72121 LUMO: -0.66668 factor:1 | 1 (-0.84978) | -1 | -1 |
| G: -5683.64846 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.39358 HOMO: -6.52257 LUMO: -0.19320 factor:1 | 1 (-1.37943) | -1 | -1 |
| G: -5683.64846 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.36294 HOMO: -6.28039 LUMO: -0.27211 factor:1 | 1 (-1.34879) | -1 | -1 |
| G: -5683.64846 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.65718 HOMO: -6.71849 LUMO: -0.42722 factor:1 | 1 (-0.64303) | -1 | -1 |
| G: -5683.64846 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.21834 HOMO: -6.27495 LUMO: 0.27756 factor:1 | 1 (-1.20419) | -1 | -1 |
| G: -5683.64846 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.48534 HOMO: -6.21780 LUMO: 0.46531 factor:1 | 1 (-0.47119) | -1 | -1 |
| G: -5683.64846 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.28274 HOMO: -6.52257 LUMO: -0.64491 factor:1 | -1 (0.73141) | -1 | -1 |
| G: -5683.64846 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.43213 HOMO: -6.73754 LUMO: 1.83133 factor:1 | -1 (0.58202) | -1 | -1 |
| G: -5683.64846 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.89614 HOMO: -6.67223 LUMO: 1.88847 factor:1 | -1 (0.11802) | -1 | -1 |
| G: -5683.64846 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.05410 HOMO: -6.82189 LUMO: 1.59187 factor:1 | 1 (-0.03995) | -1 | -1 |
| G: -5683.64846 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.00836 HOMO: -6.43277 LUMO: 1.76330 factor:1 | -1 (0.00580) | -1 | -1 |
| G: -5683.64846 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.13894 HOMO: -6.48175 LUMO: 1.77962 factor:1 | 1 (-0.12479) | -1 | -1 |
| G: -5683.64846 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11946.20955 HOMO: -6.50352 LUMO: 1.68438 factor:1 | -1 (1.80460) | -1 | -1 |
| G: -5683.64846 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.03198 HOMO: -6.31576 LUMO: 2.03813 factor:1 | -1 (0.98217) | -1 | -1 |
| G: -5683.64846 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.57092 HOMO: -6.27495 LUMO: 1.99459 factor:1 | 1 (-0.55677) | -1 | -1 |
| G: -5683.64846 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.77300 HOMO: -6.23957 LUMO: 2.17147 factor:1 | 1 (-0.75884) | -1 | -1 |
| G: -5683.64846 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.94537 HOMO: -6.78108 LUMO: 2.16875 factor:1 | 1 (-1.93122) | -1 | -1 |
| G: -5683.64846 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.93174 HOMO: -6.34297 LUMO: 2.10344 factor:1 | 1 (-1.91759) | -1 | -1 |
| G: -5683.64846 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.85602 HOMO: -6.30216 LUMO: 2.00004 factor:1 | 1 (-0.84187) | -1 | -1 |
| G: -5683.64846 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.50017 HOMO: -6.72665 LUMO: 2.09528 factor:1 | 1 (-1.48601) | -1 | -1 |
| G: -5683.64846 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.19624 HOMO: -6.86543 LUMO: 1.91568 factor:1 | 1 (-1.18209) | -1 | -1 |
| G: -5683.64846 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.93382 HOMO: -5.83956 LUMO: 1.89391 factor:1 | 1 (-0.91966) | -1 | -1 |
| G: -5683.64846 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.81558 HOMO: -6.42189 LUMO: 2.03269 factor:1 | 1 (-0.80143) | -1 | -1 |
| G: -5683.64846 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.64381 HOMO: -6.07630 LUMO: 1.80956 factor:1 | 1 (-1.62966) | -1 | -1 |
| G: -5683.64846 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.15670 HOMO: -6.43277 LUMO: 1.81772 factor:1 | 1 (-1.14255) | -1 | -1 |
| G: -5683.64846 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.90170 HOMO: -7.03959 LUMO: 1.78779 factor:1 | 1 (-1.88755) | -1 | -1 |
| G: -5683.64846 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.98334 HOMO: -6.72121 LUMO: 2.29664 factor:1 | 1 (-0.96919) | -1 | -1 |
| G: -5683.64846 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.76592 HOMO: -6.62869 LUMO: 2.04630 factor:1 | 1 (-0.75177) | -1 | -1 |
| G: -5683.64846 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.92152 HOMO: -6.63958 LUMO: 1.84221 factor:1 | -1 (0.09263) | -1 | -1 |
| G: -5683.64846 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.96041 HOMO: -6.70761 LUMO: 1.67350 factor:1 | -1 (0.05374) | -1 | -1 |
| G: -5683.64846 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.80021 HOMO: -6.00283 LUMO: 1.64357 factor:1 | 1 (-0.78606) | -1 | -1 |
| G: -5683.64846 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.03351 HOMO: -6.48719 LUMO: 1.70343 factor:1 | -1 (0.98064) | -1 | -1 |
| G: -5683.64846 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.60076 HOMO: -6.13345 LUMO: 1.44492 factor:1 | -1 (0.41340) | -1 | -1 |
| G: -5683.64846 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.73660 HOMO: -6.11168 LUMO: 1.70071 factor:1 | -1 (0.27756) | -1 | -1 |
| G: -5683.64846 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11946.53363 HOMO: -6.09535 LUMO: 1.82316 factor:1 | -1 (1.48052) | -1 | -1 |
| G: -5683.64846 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11946.28781 HOMO: -6.81101 LUMO: 1.63540 factor:1 | -1 (1.72634) | -1 | -1 |
| G: -5683.64846 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.50671 HOMO: -6.80013 LUMO: 2.12249 factor:1 | 1 (-0.49255) | -1 | -1 |
| G: -5683.64846 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.57175 HOMO: -6.48447 LUMO: 1.94561 factor:1 | -1 (0.44240) | -1 | -1 |
| G: -5683.64846 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.61503 HOMO: -6.72393 LUMO: 2.06534 factor:1 | 1 (-0.60088) | -1 | -1 |
| G: -5683.64846 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.62878 HOMO: -6.34570 LUMO: 1.98915 factor:1 | -1 (0.38537) | -1 | -1 |
| G: -5683.64846 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.76116 HOMO: -6.31304 LUMO: 1.87759 factor:1 | 1 (-0.74701) | -1 | -1 |
| G: -5683.64846 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.86384 HOMO: -6.77564 LUMO: 1.81228 factor:1 | -1 (0.15032) | -1 | -1 |
| G: -5683.64846 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.84225 HOMO: -6.58516 LUMO: 2.34834 factor:1 | 1 (-0.82810) | -1 | -1 |
| G: -5683.64846 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.91055 HOMO: -6.68040 LUMO: 2.20412 factor:1 | 1 (-0.89640) | -1 | -1 |
| G: -5683.64846 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.30245 HOMO: -6.20964 LUMO: 2.17147 factor:1 | 1 (-1.28830) | -1 | -1 |
| G: -5683.64846 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.02701 HOMO: -6.54706 LUMO: 2.03813 factor:1 | 1 (-2.01285) | -1 | -1 |
| G: -5683.64846 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.80624 HOMO: -6.54162 LUMO: 2.17419 factor:1 | 1 (-1.79209) | -1 | -1 |
| G: -5683.64846 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.49953 HOMO: -6.75659 LUMO: 2.22589 factor:1 | 1 (-2.48538) | -1 | -1 |
| G: -5683.64846 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.65886 HOMO: -6.59604 LUMO: 2.59325 factor:1 | 1 (-1.64471) | -1 | -1 |
| G: -5683.64846 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.43518 HOMO: -6.11712 LUMO: 2.02181 factor:1 | 1 (-2.42102) | -1 | -1 |
| G: -5683.64846 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.89187 HOMO: -6.63141 LUMO: 2.09256 factor:1 | 1 (-1.87772) | -1 | -1 |
| G: -5683.64846 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.31401 HOMO: -6.61781 LUMO: 1.86126 factor:1 | 1 (-1.29986) | -1 | -1 |
| G: -5683.64846 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.97811 HOMO: -6.63958 LUMO: 1.77146 factor:1 | 1 (-1.96395) | -1 | -1 |
| G: -5683.64846 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.02989 HOMO: -6.60420 LUMO: 1.54561 factor:1 | 1 (-2.01574) | -1 | -1 |
| G: -5683.64846 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.30726 HOMO: -6.52529 LUMO: 2.05174 factor:1 | 1 (-1.29311) | -1 | -1 |
| G: -5683.64846 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.80364 HOMO: -6.80285 LUMO: 2.13609 factor:1 | -1 (0.21051) | -1 | -1 |
| G: -5683.64846 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.66304 HOMO: -6.51168 LUMO: 2.25855 factor:1 | -1 (0.35111) | -1 | -1 |
| G: -5683.64846 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.05212 HOMO: -6.64774 LUMO: 2.46263 factor:1 | -1 (0.96203) | -1 | -1 |
| G: -5683.64846 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.66837 HOMO: -6.40828 LUMO: 1.99732 factor:1 | 1 (-0.65422) | -1 | -1 |
| G: -5683.64846 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.90359 HOMO: -5.97562 LUMO: 1.56465 factor:1 | -1 (0.11056) | -1 | -1 |
| G: -5683.64846 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.95274 HOMO: -6.75659 LUMO: 2.23405 factor:1 | -1 (0.06142) | -1 | -1 |
| G: -5683.64846 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.00231 HOMO: -6.68584 LUMO: 2.09528 factor:1 | -1 (0.01184) | -1 | -1 |
| G: -5683.64846 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.88742 HOMO: -6.86543 LUMO: 1.95106 factor:1 | 1 (-0.87327) | -1 | -1 |
| G: -5683.64846 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.91090 HOMO: -6.47359 LUMO: 1.82316 factor:1 | 1 (-0.89675) | -1 | -1 |
| G: -5683.64846 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.91305 HOMO: -6.87632 LUMO: 2.08439 factor:1 | 1 (-0.89890) | -1 | -1 |
| G: -5683.64846 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.86564 HOMO: -6.33753 LUMO: 2.16603 factor:1 | 1 (-1.85149) | -1 | -1 |
| G: -5683.64846 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.12332 HOMO: -6.92258 LUMO: 1.72248 factor:1 | 1 (-1.10916) | -1 | -1 |
| G: -5683.64846 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.59976 HOMO: -6.62597 LUMO: 2.10344 factor:1 | 1 (-1.58561) | -1 | -1 |
| G: -5683.64846 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.84995 HOMO: -6.63141 LUMO: 1.94017 factor:1 | 1 (-0.83580) | -1 | -1 |
| G: -5683.64846 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.81467 HOMO: -6.48447 LUMO: 1.91840 factor:1 | 1 (-1.80052) | -1 | -1 |
| G: -5683.64846 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.08604 HOMO: -6.41372 LUMO: 1.61364 factor:1 | 1 (-1.07188) | -1 | -1 |
| G: -5683.64846 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.91338 HOMO: -6.37291 LUMO: 1.79051 factor:1 | 1 (-0.89923) | -1 | -1 |
| G: -5683.64846 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.99977 HOMO: -6.13073 LUMO: 1.77962 factor:1 | 1 (-1.98561) | -1 | -1 |
| G: -5683.64846 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.27711 HOMO: -6.13073 LUMO: 1.98915 factor:1 | 1 (-1.26296) | -1 | -1 |
| G: -5683.64846 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.04040 HOMO: -6.44094 LUMO: 1.58370 factor:1 | 1 (-1.02625) | -1 | -1 |
| G: -5683.64846 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.88595 HOMO: -6.87087 LUMO: -0.82995 factor:1 | 1 (-0.87180) | -1 | -1 |
| G: -5683.64846 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.15990 HOMO: -6.67223 LUMO: 1.08029 factor:1 | -1 (0.85425) | -1 | -1 |
| G: -5683.64846 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.39346 HOMO: -6.82462 LUMO: 0.91702 factor:1 | -1 (0.62069) | -1 | -1 |
| G: -5683.64846 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.36519 HOMO: -6.65863 LUMO: 1.52656 factor:1 | -1 (0.64896) | -1 | -1 |
| G: -5683.64846 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.31269 HOMO: -6.78924 LUMO: 0.86260 factor:1 | 1 (-0.29854) | -1 | -1 |
| G: -5683.64846 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11946.26383 HOMO: -6.68584 LUMO: 0.94424 factor:1 | -1 (1.75032) | -1 | -1 |
| G: -5683.64846 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.35924 HOMO: -6.58788 LUMO: 1.00138 factor:1 | 1 (-1.34509) | -1 | -1 |
| G: -5683.64846 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.46055 HOMO: -6.79740 LUMO: 0.91430 factor:1 | 1 (-1.44639) | -1 | -1 |
| G: -5683.64846 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.58734 HOMO: -6.67223 LUMO: 0.80274 factor:1 | -1 (0.42681) | -1 | -1 |
| G: -5683.64846 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.47798 HOMO: -6.95251 LUMO: 0.90614 factor:1 | -1 (0.53617) | -1 | -1 |
| G: -5683.64846 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.34576 HOMO: -7.19469 LUMO: 1.34152 factor:1 | -1 (0.66839) | -1 | -1 |
| G: -5683.64846 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.40747 HOMO: -6.59332 LUMO: -0.76464 factor:1 | -1 (0.60668) | -1 | -1 |
| G: -5683.64846 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.08454 HOMO: -6.77564 LUMO: -0.90886 factor:1 | 1 (-1.07039) | -1 | -1 |
| G: -5683.64846 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.73089 HOMO: -6.57971 LUMO: -0.41633 factor:1 | 1 (-1.71674) | -1 | -1 |
| G: -5683.64846 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.08739 HOMO: -6.68856 LUMO: -0.58232 factor:1 | 1 (-2.07324) | -1 | -1 |
| G: -5683.64846 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.85329 HOMO: -6.87087 LUMO: -0.71022 factor:1 | 1 (-1.83914) | -1 | -1 |
| G: -5683.64846 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.24941 HOMO: -6.67767 LUMO: -0.74559 factor:1 | 1 (-1.23526) | -1 | -1 |
| G: -5683.64846 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.97247 HOMO: -6.68040 LUMO: -0.65307 factor:1 | 1 (-1.95832) | -1 | -1 |
| G: -5683.64846 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.93917 HOMO: -6.32937 LUMO: 0.80274 factor:1 | 1 (-1.92502) | -1 | -1 |
| G: -5683.64846 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.34648 HOMO: -6.29671 LUMO: 0.82723 factor:1 | 1 (-1.33232) | -1 | -1 |
| G: -5683.64846 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.92978 HOMO: -6.67767 LUMO: 0.59321 factor:1 | 1 (-1.91563) | -1 | -1 |
| G: -5683.64846 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.06129 HOMO: -6.77836 LUMO: 0.50341 factor:1 | 1 (-2.04714) | -1 | -1 |
| G: -5683.64846 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.49279 HOMO: -6.61781 LUMO: 0.42450 factor:1 | 1 (-1.47864) | -1 | -1 |
| G: -5683.64846 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.97076 HOMO: -6.83278 LUMO: 0.39457 factor:1 | 1 (-1.95661) | -1 | -1 |
| G: -5683.64846 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.69035 HOMO: -6.56883 LUMO: 0.64219 factor:1 | 1 (-1.67619) | -1 | -1 |
| G: -5683.64846 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.07536 HOMO: -6.71577 LUMO: 0.40001 factor:1 | -1 (0.93879) | -1 | -1 |
| G: -5683.64846 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.20921 HOMO: -6.86543 LUMO: -0.74287 factor:1 | -1 (0.80494) | -1 | -1 |
| G: -5683.64846 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.72041 HOMO: -6.68584 LUMO: -0.69389 factor:1 | 1 (-2.70625) | -1 | -1 |
| G: -5683.64846 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.01862 HOMO: -6.61237 LUMO: -0.48980 factor:1 | 1 (-2.00447) | -1 | -1 |
| G: -5683.64846 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.82805 HOMO: -6.80285 LUMO: -0.58232 factor:1 | 1 (-2.81390) | -1 | -1 |
| G: -5683.64846 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.00913 HOMO: -6.88992 LUMO: -0.70205 factor:1 | 1 (-1.99498) | -1 | -1 |
| G: -5683.64846 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.66205 HOMO: -6.95251 LUMO: -0.71838 factor:1 | 1 (-1.64789) | -1 | -1 |
| G: -5683.64846 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.69454 HOMO: -7.52123 LUMO: 0.27211 factor:1 | 1 (-1.68038) | -1 | -1 |
| G: -5683.64846 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.49156 HOMO: -6.76747 LUMO: -0.74015 factor:1 | 1 (-2.47741) | -1 | -1 |
| G: -5683.64846 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.94659 HOMO: -6.55250 LUMO: -0.49797 factor:1 | 1 (-2.93244) | -1 | -1 |
| G: -5683.64846 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.39384 HOMO: -6.50896 LUMO: -0.46804 factor:1 | 1 (-2.37969) | -1 | -1 |
| G: -5683.64846 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.39475 HOMO: -7.45320 LUMO: 0.08436 factor:1 | 1 (-1.38060) | -1 | -1 |
| G: -5683.64846 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.76727 HOMO: -6.82462 LUMO: -0.70477 factor:1 | 1 (-1.75312) | -1 | -1 |
| G: -5683.64846 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.61505 HOMO: -6.57155 LUMO: -0.43538 factor:1 | 1 (-1.60090) | -1 | -1 |
| G: -5683.64846 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.60888 HOMO: -6.72665 LUMO: -0.55239 factor:1 | 1 (-1.59472) | -1 | -1 |
| G: -5683.64846 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.26557 HOMO: -7.05319 LUMO: -1.08573 factor:1 | 1 (-2.25142) | -1 | -1 |
| G: -5683.64846 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.50720 HOMO: -6.56067 LUMO: -0.45715 factor:1 | 1 (-2.49305) | -1 | -1 |
| G: -5683.64846 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11951.09824 HOMO: -6.76475 LUMO: -0.53879 factor:1 | 1 (-3.08408) | -1 | -1 |
| G: -5683.64846 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.16791 HOMO: -6.67223 LUMO: -0.45987 factor:1 | 1 (-2.15375) | -1 | -1 |
| G: -5683.64846 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.04125 HOMO: -6.44094 LUMO: -0.72110 factor:1 | 1 (-1.02709) | -1 | -1 |
| G: -5683.64846 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.33546 HOMO: -6.66951 LUMO: -0.67756 factor:1 | 1 (-1.32130) | -1 | -1 |
| G: -5683.64846 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.04556 HOMO: -6.69400 LUMO: -0.62858 factor:1 | 1 (-2.03141) | -1 | -1 |
| G: -5683.64846 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.99438 HOMO: -6.51985 LUMO: -0.37007 factor:1 | 1 (-1.98023) | -1 | -1 |
| G: -5683.64846 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.09466 HOMO: -5.98378 LUMO: 0.78641 factor:1 | 1 (-1.08051) | -1 | -1 |
| G: -5683.64846 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.10402 HOMO: -6.11440 LUMO: 0.71294 factor:1 | 1 (-1.08987) | -1 | -1 |
| G: -5683.64846 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.05940 HOMO: -6.45182 LUMO: 0.63947 factor:1 | 1 (-1.04524) | -1 | -1 |
| G: -5683.64846 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.73836 HOMO: -6.78924 LUMO: 0.37007 factor:1 | 1 (-0.72420) | -1 | -1 |
| G: -5683.64846 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.91364 HOMO: -6.63686 LUMO: 0.54423 factor:1 | 1 (-1.89949) | -1 | -1 |
| G: -5683.64846 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.04084 HOMO: -6.66679 LUMO: 0.48708 factor:1 | 1 (-1.02669) | -1 | -1 |
| G: -5683.64846 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.21680 HOMO: -6.81917 LUMO: 0.31021 factor:1 | 1 (-2.20265) | -1 | -1 |
| G: -5683.64846 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.93027 HOMO: -6.28583 LUMO: 0.44899 factor:1 | 1 (-1.91612) | -1 | -1 |
| G: -5683.64846 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.42459 HOMO: -6.61237 LUMO: 0.49525 factor:1 | 1 (-2.41044) | -1 | -1 |
| G: -5683.64846 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.97759 HOMO: -7.08857 LUMO: 0.38368 factor:1 | 1 (-1.96344) | -1 | -1 |
| G: -5683.64846 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.51126 HOMO: -6.53890 LUMO: -0.68845 factor:1 | 1 (-2.49711) | -1 | -1 |
| G: -5683.64846 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.91092 HOMO: -6.56611 LUMO: -0.66396 factor:1 | 1 (-1.89677) | -1 | -1 |
| G: -5683.64846 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.19123 HOMO: -6.04909 LUMO: -0.59865 factor:1 | 1 (-2.17707) | -1 | -1 |
| G: -5683.64846 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.05006 HOMO: -6.74842 LUMO: -0.77825 factor:1 | 1 (-1.03591) | -1 | -1 |
| G: -5683.64846 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.87253 HOMO: -6.82462 LUMO: -0.61498 factor:1 | 1 (-1.85837) | -1 | -1 |
| G: -5683.64846 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.07574 HOMO: -7.40694 LUMO: 0.32926 factor:1 | 1 (-2.06159) | -1 | -1 |
| G: -5683.64846 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.02410 HOMO: -6.80557 LUMO: -0.57416 factor:1 | 1 (-1.00995) | -1 | -1 |
| G: -5683.64846 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.96990 HOMO: -6.76747 LUMO: -0.67484 factor:1 | 1 (-0.95575) | -1 | -1 |
| G: -5683.64846 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.12881 HOMO: -7.23279 LUMO: 0.48980 factor:1 | 1 (-1.11466) | -1 | -1 |
| G: -5683.64846 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.61993 HOMO: -6.62869 LUMO: -0.24762 factor:1 | 1 (-0.60578) | -1 | -1 |
| G: -5683.64846 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.00772 HOMO: -6.65863 LUMO: -0.28028 factor:1 | 1 (-0.99357) | -1 | -1 |
| G: -5683.64846 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.22500 HOMO: -6.50352 LUMO: -0.44899 factor:1 | 1 (-2.21084) | -1 | -1 |
| G: -5683.64846 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.05120 HOMO: -6.62053 LUMO: -0.88437 factor:1 | 1 (-1.03705) | -1 | -1 |
| G: -5683.64846 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.20695 HOMO: -6.73754 LUMO: -0.77825 factor:1 | 1 (-2.19280) | -1 | -1 |
| G: -5683.64846 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.75535 HOMO: -7.24639 LUMO: 0.35647 factor:1 | 1 (-1.74120) | -1 | -1 |
| G: -5683.64846 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.95264 HOMO: -6.46270 LUMO: -0.48164 factor:1 | 1 (-1.93848) | -1 | -1 |
| G: -5683.64846 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.34607 HOMO: -6.14161 LUMO: -0.66396 factor:1 | 1 (-1.33192) | -1 | -1 |
| G: -5683.64846 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.55433 HOMO: -6.63414 LUMO: 1.51295 factor:1 | 1 (-2.54018) | -1 | -1 |
| G: -5683.64846 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.01571 HOMO: -6.52529 LUMO: 1.65989 factor:1 | 1 (-2.00156) | -1 | -1 |
| G: -5683.64846 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.42443 HOMO: -6.63686 LUMO: 1.64629 factor:1 | 1 (-2.41028) | -1 | -1 |
| G: -5683.64846 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.32566 HOMO: -6.49808 LUMO: 1.60003 factor:1 | 1 (-1.31151) | -1 | -1 |
| G: -5683.64846 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.17144 HOMO: -6.85183 LUMO: 1.96194 factor:1 | 1 (-2.15729) | -1 | -1 |
| G: -5683.64846 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.24782 HOMO: -6.90081 LUMO: 1.82316 factor:1 | 1 (-0.23366) | -1 | -1 |
| G: -5683.64846 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.94832 HOMO: -6.20147 LUMO: 1.95106 factor:1 | 1 (-0.93417) | -1 | -1 |
| G: -5683.64846 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.60586 HOMO: -7.05047 LUMO: 1.94289 factor:1 | 1 (-0.59171) | -1 | -1 |
| G: -5683.64846 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.81659 HOMO: -6.11440 LUMO: 1.83949 factor:1 | 1 (-0.80244) | -1 | -1 |
| G: -5683.64846 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.71713 HOMO: -6.65046 LUMO: 1.59187 factor:1 | 1 (-0.70298) | -1 | -1 |
| G: -5683.64846 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.17590 HOMO: -6.81917 LUMO: 2.41365 factor:1 | 1 (-0.16174) | -1 | -1 |
| G: -5683.64846 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.91041 HOMO: -6.40284 LUMO: 2.48984 factor:1 | 1 (-0.89626) | -1 | -1 |
| G: -5683.64846 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.50927 HOMO: -7.04775 LUMO: 2.31025 factor:1 | 1 (-2.49512) | -1 | -1 |
| G: -5683.64846 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.51143 HOMO: -6.64774 LUMO: 2.20140 factor:1 | 1 (-1.49728) | -1 | -1 |
| G: -5683.64846 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.08728 HOMO: -6.72393 LUMO: 2.28304 factor:1 | 1 (-2.07313) | -1 | -1 |
| G: -5683.64846 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.09465 HOMO: -6.35114 LUMO: 1.84765 factor:1 | 1 (-2.08050) | -1 | -1 |
| G: -5683.64846 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.48175 HOMO: -6.41100 LUMO: 1.74697 factor:1 | 1 (-0.46760) | -1 | -1 |
| G: -5683.64846 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.06418 HOMO: -6.34297 LUMO: 1.55921 factor:1 | 1 (-1.05003) | -1 | -1 |
| G: -5683.64846 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.01003 HOMO: -6.31848 LUMO: 1.67622 factor:1 | 1 (-0.99588) | -1 | -1 |
| G: -5683.64846 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.30452 HOMO: -6.50896 LUMO: 2.02725 factor:1 | 1 (-1.29036) | -1 | -1 |
| G: -5683.64846 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.68268 HOMO: -6.28583 LUMO: 2.00548 factor:1 | 1 (-0.66853) | -1 | -1 |
| G: -5683.64846 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.21616 HOMO: -6.67495 LUMO: 1.92384 factor:1 | 1 (-1.20201) | -1 | -1 |
| G: -5683.64846 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.85375 HOMO: -6.17154 LUMO: 2.39732 factor:1 | 1 (-1.83960) | -1 | -1 |
| G: -5683.64846 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.12247 HOMO: -6.84911 LUMO: 2.24766 factor:1 | 1 (-1.10832) | -1 | -1 |
| G: -5683.64846 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.68575 HOMO: -6.77564 LUMO: 2.38372 factor:1 | 1 (-1.67160) | -1 | -1 |
| G: -5683.64846 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.95839 HOMO: -6.18243 LUMO: 2.40821 factor:1 | 1 (-0.94424) | -1 | -1 |
| G: -5683.64846 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.18960 HOMO: -6.40828 LUMO: 2.22589 factor:1 | 1 (-1.17545) | -1 | -1 |
| G: -5683.64846 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.05504 HOMO: -6.74570 LUMO: 1.88303 factor:1 | 1 (-1.04089) | -1 | -1 |
| G: -5683.64846 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.81574 HOMO: -6.29944 LUMO: 2.05174 factor:1 | 1 (-1.80158) | -1 | -1 |
| G: -5683.64846 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.04872 HOMO: -7.00693 LUMO: 2.16331 factor:1 | 1 (-2.03457) | -1 | -1 |
| G: -5683.64846 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.01461 HOMO: -6.89537 LUMO: 2.19596 factor:1 | 1 (-1.00045) | -1 | -1 |
| G: -5683.64846 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.76953 HOMO: -6.72665 LUMO: 2.03813 factor:1 | 1 (-1.75538) | -1 | -1 |
| G: -5683.64846 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.56596 HOMO: -6.69944 LUMO: 2.36467 factor:1 | 1 (-1.55181) | -1 | -1 |
| G: -5683.64846 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.96194 HOMO: -6.92802 LUMO: 1.72792 factor:1 | 1 (-1.94779) | -1 | -1 |
| G: -5683.64846 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.55116 HOMO: -6.12256 LUMO: 1.85310 factor:1 | 1 (-1.53701) | -1 | -1 |
| G: -5683.64846 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.09583 HOMO: -6.70489 LUMO: 2.20956 factor:1 | 1 (-1.08168) | -1 | -1 |
| G: -5683.64846 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.06541 HOMO: -6.94707 LUMO: 1.81500 factor:1 | 1 (-1.05126) | -1 | -1 |
| G: -5683.64846 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.93588 HOMO: -6.39468 LUMO: 1.79051 factor:1 | 1 (-0.92173) | -1 | -1 |
| G: -5683.64846 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.80330 HOMO: -6.69128 LUMO: 2.03813 factor:1 | 1 (-1.78915) | -1 | -1 |
| G: -5683.64846 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.39885 HOMO: -6.55250 LUMO: 2.00548 factor:1 | 1 (-2.38470) | -1 | -1 |
| G: -5683.64846 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.59568 HOMO: -6.24773 LUMO: 2.09256 factor:1 | 1 (-1.58153) | -1 | -1 |
| G: -5683.64846 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.08657 HOMO: -6.85727 LUMO: 1.70071 factor:1 | 1 (-2.07242) | -1 | -1 |
| G: -5683.64846 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.49014 HOMO: -6.71305 LUMO: 1.72520 factor:1 | 1 (-2.47599) | -1 | -1 |
| G: -5683.64846 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.16799 HOMO: -6.81101 LUMO: 2.15514 factor:1 | 1 (-2.15384) | -1 | -1 |
| G: -5683.64846 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.94036 HOMO: -6.93618 LUMO: 1.75513 factor:1 | 1 (-2.92620) | -1 | -1 |
| G: -5683.64846 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.98262 HOMO: -6.63686 LUMO: 2.09800 factor:1 | 1 (-1.96847) | -1 | -1 |
| G: -5683.64846 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11951.50858 HOMO: -6.98244 LUMO: 1.72520 factor:1 | 1 (-3.49443) | -1 | -1 |
| G: -5683.64846 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.89207 HOMO: -6.37019 LUMO: 2.35923 factor:1 | 1 (-0.87792) | -1 | -1 |
| G: -5683.64846 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.95945 HOMO: -6.55794 LUMO: 2.12521 factor:1 | 1 (-0.94530) | -1 | -1 |
| G: -5683.64846 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.04459 HOMO: -6.45998 LUMO: 1.93201 factor:1 | 1 (-1.03044) | -1 | -1 |
| G: -5683.64846 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.46258 HOMO: -6.71033 LUMO: 1.58370 factor:1 | 1 (-2.44843) | -1 | -1 |
| G: -5683.64846 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.02156 HOMO: -6.67223 LUMO: 1.52928 factor:1 | 1 (-2.00741) | -1 | -1 |
| G: -5683.64846 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.35060 HOMO: -6.72121 LUMO: 1.33608 factor:1 | 1 (-2.33645) | -1 | -1 |
| G: -5683.64846 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.32037 HOMO: -6.89264 LUMO: 2.08983 factor:1 | 1 (-2.30622) | -1 | -1 |
| G: -5683.64846 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11951.64304 HOMO: -6.31032 LUMO: 2.24766 factor:1 | 1 (-3.62888) | -1 | -1 |
| G: -5683.64846 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.88966 HOMO: -6.79740 LUMO: 2.09528 factor:1 | 1 (-2.87551) | -1 | -1 |
| G: -5683.64846 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.98789 HOMO: -6.78108 LUMO: 2.15786 factor:1 | 1 (-2.97374) | -1 | -1 |
| G: -5683.64846 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.07847 HOMO: -6.50896 LUMO: 2.15786 factor:1 | 1 (-1.06432) | -1 | -1 |
| G: -5683.64846 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.10685 HOMO: -6.56067 LUMO: 2.24494 factor:1 | 1 (-1.09270) | -1 | -1 |
| G: -5683.64846 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.76061 HOMO: -6.72938 LUMO: 2.24494 factor:1 | 1 (-0.74646) | -1 | -1 |
| G: -5683.64846 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.92005 HOMO: -6.40556 LUMO: 1.58642 factor:1 | 1 (-0.90589) | -1 | -1 |
| G: -5683.64846 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.73359 HOMO: -6.63141 LUMO: 1.66262 factor:1 | 1 (-0.71944) | -1 | -1 |
| G: -5683.64846 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11945.57944 HOMO: -6.97156 LUMO: 2.23678 factor:1 | -1 (2.43471) | -1 | -1 |
| G: -5683.64846 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.42093 HOMO: -6.86271 LUMO: 1.91296 factor:1 | 1 (-0.40678) | -1 | -1 |
| G: -5683.64846 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.01735 HOMO: -6.50624 LUMO: 1.89119 factor:1 | 1 (-1.00320) | -1 | -1 |
| G: -5683.64846 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11946.70760 HOMO: -6.70761 LUMO: 1.56193 factor:1 | -1 (1.30655) | -1 | -1 |
| G: -5683.64846 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11946.65239 HOMO: -6.60420 LUMO: 1.79595 factor:1 | -1 (1.36177) | -1 | -1 |
| G: -5683.64846 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11946.62727 HOMO: -6.85727 LUMO: 2.26943 factor:1 | -1 (1.38688) | -1 | -1 |
| G: -5683.64846 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.80679 HOMO: -6.23413 LUMO: 1.91024 factor:1 | 1 (-0.79264) | -1 | -1 |
| G: -5683.64846 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.09112 HOMO: -6.84366 LUMO: 2.01364 factor:1 | 1 (-1.07697) | -1 | -1 |
| G: -5683.64846 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.44937 HOMO: -6.63414 LUMO: 2.54971 factor:1 | 1 (-0.43522) | -1 | -1 |
| G: -5683.64846 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.29837 HOMO: -6.52257 LUMO: 2.42998 factor:1 | 1 (-0.28422) | -1 | -1 |
| G: -5683.64846 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.76638 HOMO: -6.61509 LUMO: 2.31297 factor:1 | 1 (-0.75223) | -1 | -1 |
| G: -5683.64846 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.86783 HOMO: -6.45998 LUMO: 2.23405 factor:1 | 1 (-0.85368) | -1 | -1 |
| G: -5683.64846 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.31834 HOMO: -6.86271 LUMO: 2.22317 factor:1 | 1 (-1.30419) | -1 | -1 |
| G: -5683.64846 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.67351 HOMO: -6.84366 LUMO: 2.11432 factor:1 | 1 (-0.65936) | -1 | -1 |
| G: -5683.64846 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.34134 HOMO: -6.85999 LUMO: 2.44902 factor:1 | 1 (-0.32719) | -1 | -1 |
| G: -5683.64846 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.73803 HOMO: -6.73482 LUMO: 1.93745 factor:1 | 1 (-0.72388) | -1 | -1 |
| G: -5683.64846 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.21527 HOMO: -6.91441 LUMO: 2.32385 factor:1 | 1 (-0.20112) | -1 | -1 |
| G: -5683.64846 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.31783 HOMO: -6.16066 LUMO: 2.26399 factor:1 | 1 (-0.30368) | -1 | -1 |
| G: -5683.64846 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.00704 HOMO: -6.71305 LUMO: 2.38644 factor:1 | 1 (-0.99289) | -1 | -1 |
| G: -5683.64846 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11944.33751 HOMO: -7.08312 LUMO: 2.01636 factor:1 | -1 (3.67664) | 1 | 1 |
| G: -5683.64846 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.07934 HOMO: -6.15249 LUMO: 1.90752 factor:1 | 1 (-1.06519) | -1 | -1 |
| G: -5683.64846 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.56339 HOMO: -6.83006 LUMO: 2.25855 factor:1 | 1 (-0.54923) | -1 | -1 |
| G: -5683.64846 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.70731 HOMO: -6.77836 LUMO: 2.24766 factor:1 | 1 (-0.69316) | -1 | -1 |
| G: -5683.64846 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.01287 HOMO: -6.66951 LUMO: 2.35923 factor:1 | -1 (0.00128) | -1 | -1 |
| G: -5683.64846 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.12451 HOMO: -6.68312 LUMO: 2.30208 factor:1 | 1 (-1.11036) | -1 | -1 |
| G: -5683.64846 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.54094 HOMO: -6.49808 LUMO: 2.49801 factor:1 | 1 (-0.52679) | -1 | -1 |
| G: -5683.64846 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.80794 HOMO: -6.62325 LUMO: 1.89935 factor:1 | 1 (-0.79378) | -1 | -1 |
| G: -5683.64846 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11946.53965 HOMO: -6.80829 LUMO: 1.91296 factor:1 | -1 (1.47450) | -1 | -1 |
| G: -5683.64846 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11946.80749 HOMO: -6.64230 LUMO: 2.13065 factor:1 | -1 (1.20666) | -1 | -1 |
| G: -5683.64846 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.05178 HOMO: -6.40556 LUMO: 1.83949 factor:1 | 1 (-1.03762) | -1 | -1 |
| G: -5683.64846 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.99662 HOMO: -6.48175 LUMO: 1.72248 factor:1 | 1 (-0.98247) | -1 | -1 |
| G: -5683.64846 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.98589 HOMO: -6.61781 LUMO: 2.11432 factor:1 | 1 (-1.97174) | -1 | -1 |
| G: -5683.64846 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.01969 HOMO: -6.34570 LUMO: 2.22317 factor:1 | 1 (-2.00553) | -1 | -1 |
| G: -5683.64846 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.37037 HOMO: -7.00149 LUMO: 1.80139 factor:1 | 1 (-1.35622) | -1 | -1 |
| G: -5683.64846 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.74246 HOMO: -6.66951 LUMO: 2.13065 factor:1 | 1 (-0.72831) | -1 | -1 |
| G: -5683.64846 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.17641 HOMO: -6.54434 LUMO: 2.20140 factor:1 | 1 (-0.16226) | -1 | -1 |
| G: -5683.64846 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.57950 HOMO: -6.67767 LUMO: 2.02997 factor:1 | -1 (0.43465) | -1 | -1 |
| G: -5683.64846 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.04725 HOMO: -6.49536 LUMO: 2.42998 factor:1 | 1 (-2.03310) | -1 | -1 |
| G: -5683.64846 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.50583 HOMO: -6.70761 LUMO: 2.71025 factor:1 | 1 (-1.49167) | -1 | -1 |
| G: -5683.64846 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.64830 HOMO: -6.62869 LUMO: 2.11160 factor:1 | 1 (-1.63415) | -1 | -1 |
| G: -5683.64846 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.72505 HOMO: -6.61781 LUMO: 2.24494 factor:1 | 1 (-0.71090) | -1 | -1 |
| G: -5683.64846 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.15600 HOMO: -6.66135 LUMO: 2.20956 factor:1 | 1 (-0.14185) | -1 | -1 |
| G: -5683.64846 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.49722 HOMO: -6.95523 LUMO: 2.03813 factor:1 | -1 (0.51693) | -1 | -1 |
| G: -5683.64846 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.76865 HOMO: -7.11578 LUMO: 2.41365 factor:1 | -1 (0.24550) | 1 | 1 |
| G: -5683.64846 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.70530 HOMO: -6.99061 LUMO: 2.13881 factor:1 | -1 (0.30885) | -1 | -1 |
| G: -5683.64846 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.96000 HOMO: -6.43277 LUMO: 2.01364 factor:1 | -1 (0.05415) | -1 | -1 |
| G: -5683.64846 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.03306 HOMO: -6.79196 LUMO: 2.04358 factor:1 | 1 (-0.01891) | -1 | -1 |
| G: -5683.64846 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.54867 HOMO: -7.08584 LUMO: 1.99732 factor:1 | 1 (-0.53451) | 1 | 1 |
| G: -5683.64846 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.88922 HOMO: -6.46815 LUMO: 2.29936 factor:1 | 1 (-0.87506) | -1 | -1 |
| G: -5683.64846 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.03099 HOMO: -6.78108 LUMO: 1.93745 factor:1 | 1 (-1.01684) | -1 | -1 |
| G: -5683.64846 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.15507 HOMO: -6.43277 LUMO: 1.80956 factor:1 | 1 (-1.14092) | -1 | -1 |
| G: -5683.64846 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.69226 HOMO: -6.71577 LUMO: -0.81090 factor:1 | 1 (-0.67811) | -1 | -1 |
| G: -5683.64846 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.05905 HOMO: -7.14027 LUMO: -0.68028 factor:1 | 1 (-0.04490) | -1 | -1 |
| G: -5683.64846 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.04381 HOMO: -7.03414 LUMO: -0.69661 factor:1 | 1 (-0.02966) | -1 | -1 |
| G: -5683.64846 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.48051 HOMO: -6.64502 LUMO: -0.47348 factor:1 | 1 (-2.46636) | -1 | -1 |
| G: -5683.64846 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.37033 HOMO: -6.60692 LUMO: 2.12793 factor:1 | 1 (-2.35618) | -1 | -1 |
| G: -5683.64846 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.73505 HOMO: -6.66407 LUMO: 1.94561 factor:1 | 1 (-1.72090) | -1 | -1 |
| G: -5683.64846 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.15234 HOMO: -7.10217 LUMO: 1.92384 factor:1 | 1 (-2.13819) | 1 | 1 |
| G: -5683.64846 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.29749 HOMO: -6.84094 LUMO: 1.66534 factor:1 | 1 (-2.28333) | -1 | -1 |
| G: -5683.64846 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.02696 HOMO: -6.93618 LUMO: 2.13065 factor:1 | 1 (-1.01281) | -1 | -1 |
| G: -5683.64846 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.44839 HOMO: -6.60692 LUMO: 2.20684 factor:1 | 1 (-0.43424) | -1 | -1 |
| G: -5683.64846 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.09197 HOMO: -6.85727 LUMO: 2.19324 factor:1 | 1 (-1.07782) | -1 | -1 |
| G: -5683.64846 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.98459 HOMO: -6.31032 LUMO: 1.76330 factor:1 | 1 (-0.97044) | -1 | -1 |
| G: -5683.64846 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.16666 HOMO: -6.43821 LUMO: 2.10072 factor:1 | 1 (-1.15251) | -1 | -1 |
| G: -5683.64846 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.18020 HOMO: -6.42189 LUMO: 2.19596 factor:1 | 1 (-0.16604) | -1 | -1 |
| G: -5683.64846 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.05946 HOMO: -6.40556 LUMO: 2.02181 factor:1 | 1 (-0.04531) | -1 | -1 |
| G: -5683.64846 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.04432 HOMO: -6.41372 LUMO: 2.26671 factor:1 | 1 (-1.03017) | -1 | -1 |
| G: -5683.64846 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.47076 HOMO: -6.60692 LUMO: 2.09800 factor:1 | 1 (-0.45661) | -1 | -1 |
| G: -5683.64846 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.65913 HOMO: -6.75931 LUMO: 1.76602 factor:1 | 1 (-1.64498) | -1 | -1 |
| G: -5683.64846 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.90826 HOMO: -6.39195 LUMO: 1.84221 factor:1 | 1 (-0.89411) | -1 | -1 |
| G: -5683.64846 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.62042 HOMO: -6.74570 LUMO: 2.04085 factor:1 | 1 (-0.60627) | -1 | -1 |
| G: -5683.64846 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.57599 HOMO: -6.77019 LUMO: 2.16875 factor:1 | 1 (-0.56183) | -1 | -1 |
| G: -5683.64846 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.13695 HOMO: -6.15522 LUMO: 1.81772 factor:1 | 1 (-1.12280) | -1 | -1 |
| G: -5683.64846 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.57021 HOMO: -6.48175 LUMO: 2.02453 factor:1 | 1 (-1.55606) | -1 | -1 |
| G: -5683.64846 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.75830 HOMO: -6.57427 LUMO: 1.77962 factor:1 | 1 (-0.74415) | -1 | -1 |
| G: -5683.64846 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.47435 HOMO: -6.57699 LUMO: 2.42998 factor:1 | 1 (-0.46020) | -1 | -1 |
| G: -5683.64846 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.09242 HOMO: -6.35386 LUMO: 2.25310 factor:1 | 1 (-2.07827) | -1 | -1 |
| G: -5683.64846 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.25733 HOMO: -6.80013 LUMO: 2.11160 factor:1 | 1 (-1.24318) | -1 | -1 |
| G: -5683.64846 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.00896 HOMO: -6.24229 LUMO: 2.05718 factor:1 | 1 (-1.99481) | -1 | -1 |
| G: -5683.64846 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.39690 HOMO: -6.42733 LUMO: 1.76874 factor:1 | 1 (-1.38275) | -1 | -1 |
| G: -5683.64846 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.01504 HOMO: -6.56883 LUMO: 2.36195 factor:1 | 1 (-1.00089) | -1 | -1 |
| G: -5683.64846 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.97579 HOMO: -6.72665 LUMO: 2.28848 factor:1 | 1 (-1.96164) | -1 | -1 |
| G: -5683.64846 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.70906 HOMO: -6.39195 LUMO: 1.79051 factor:1 | 1 (-2.69491) | -1 | -1 |
| G: -5683.64846 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.91283 HOMO: -6.70761 LUMO: 0.15510 factor:1 | 1 (-1.89867) | -1 | -1 |
| G: -5683.64846 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.85963 HOMO: -6.44366 LUMO: -0.16871 factor:1 | 1 (-1.84548) | -1 | -1 |
| G: -5683.64846 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.65477 HOMO: -6.68584 LUMO: 1.69527 factor:1 | 1 (-2.64062) | -1 | -1 |
| G: -5683.64846 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.61923 HOMO: -6.26950 LUMO: 1.61636 factor:1 | 1 (-2.60508) | -1 | -1 |
| G: -5683.64846 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.20880 HOMO: -6.47631 LUMO: 1.98915 factor:1 | -1 (0.80535) | -1 | -1 |
| G: -5683.64846 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11946.33654 HOMO: -6.58243 LUMO: 1.97283 factor:1 | -1 (1.67761) | -1 | -1 |
| G: -5683.64846 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11946.32862 HOMO: -6.51713 LUMO: 1.97283 factor:1 | -1 (1.68553) | -1 | -1 |
| G: -5683.64846 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11946.93193 HOMO: -6.65046 LUMO: 1.69255 factor:1 | -1 (1.08222) | -1 | -1 |
| G: -5683.64846 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.03568 HOMO: -6.26406 LUMO: 2.21773 factor:1 | -1 (0.97847) | -1 | -1 |
| G: -5683.64846 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11945.98119 HOMO: -6.88992 LUMO: 2.28304 factor:1 | -1 (2.03296) | -1 | -1 |
| G: -5683.64846 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.01871 HOMO: -6.67767 LUMO: 2.34834 factor:1 | 1 (-1.00456) | -1 | -1 |
| G: -5683.64846 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.42850 HOMO: -6.52801 LUMO: 2.10344 factor:1 | 1 (-0.41435) | -1 | -1 |
| G: -5683.64846 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.93041 HOMO: -6.52801 LUMO: 2.24222 factor:1 | 1 (-0.91626) | -1 | -1 |
| G: -5683.64846 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.38444 HOMO: -6.17154 LUMO: 1.89663 factor:1 | 1 (-0.37029) | -1 | -1 |
| G: -5683.64846 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.19006 HOMO: -6.42733 LUMO: 2.15514 factor:1 | 1 (-1.17591) | -1 | -1 |
| G: -5683.64846 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.95333 HOMO: -6.36474 LUMO: 2.01364 factor:1 | -1 (0.06082) | -1 | -1 |
| G: -5683.64846 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.51950 HOMO: -6.82189 LUMO: 1.86942 factor:1 | -1 (0.49465) | -1 | -1 |
| G: -5683.64846 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.06736 HOMO: -6.60148 LUMO: 2.00548 factor:1 | -1 (0.94679) | -1 | -1 |
| G: -5683.64846 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.13800 HOMO: -6.67767 LUMO: 2.15786 factor:1 | -1 (0.87615) | -1 | -1 |
| G: -5683.64846 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.02978 HOMO: -6.79196 LUMO: 2.06534 factor:1 | -1 (0.98437) | -1 | -1 |
| G: -5683.64846 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.97939 HOMO: -6.70216 LUMO: 1.83405 factor:1 | 1 (-0.96524) | -1 | -1 |
| G: -5683.64846 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.15794 HOMO: -6.58788 LUMO: 1.79051 factor:1 | 1 (-0.14378) | -1 | -1 |
| G: -5683.64846 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.01687 HOMO: -6.34842 LUMO: 1.80139 factor:1 | 1 (-0.00272) | -1 | -1 |
| G: -5683.64846 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.08535 HOMO: -6.48175 LUMO: 1.95922 factor:1 | -1 (0.92881) | -1 | -1 |
| G: -5683.64846 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11946.98219 HOMO: -6.71033 LUMO: 2.02997 factor:1 | -1 (1.03196) | -1 | -1 |
| G: -5683.64846 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.59283 HOMO: -6.89264 LUMO: 2.42726 factor:1 | 1 (-0.57868) | -1 | -1 |
| G: -5683.64846 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.85670 HOMO: -6.74570 LUMO: 2.20684 factor:1 | 1 (-0.84255) | -1 | -1 |
| G: -5683.64846 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.06447 HOMO: -6.30216 LUMO: 2.15242 factor:1 | 1 (-0.05031) | -1 | -1 |
| G: -5683.64846 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11946.79350 HOMO: -6.94979 LUMO: 2.43814 factor:1 | -1 (1.22065) | -1 | -1 |
| G: -5683.64846 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.84363 HOMO: -6.97972 LUMO: 2.11432 factor:1 | 1 (-1.82948) | -1 | -1 |
| G: -5683.64846 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.14478 HOMO: -6.17154 LUMO: 1.98099 factor:1 | 1 (-1.13063) | -1 | -1 |
| G: -5683.64846 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.96334 HOMO: -6.74026 LUMO: 2.21501 factor:1 | 1 (-0.94919) | -1 | -1 |
| G: -5683.64846 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.12206 HOMO: -6.72393 LUMO: 2.19596 factor:1 | 1 (-1.10791) | -1 | -1 |
| G: -5683.64846 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.82355 HOMO: -6.11440 LUMO: 2.10072 factor:1 | 1 (-1.80939) | -1 | -1 |
| G: -5683.64846 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.81484 HOMO: -6.34297 LUMO: 1.92657 factor:1 | 1 (-1.80069) | -1 | -1 |
| G: -5683.64846 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.45834 HOMO: -6.24773 LUMO: 2.00276 factor:1 | 1 (-1.44419) | -1 | -1 |
| G: -5683.64846 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.64176 HOMO: -6.75114 LUMO: 1.98643 factor:1 | 1 (-0.62760) | -1 | -1 |
| G: -5683.64846 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.07701 HOMO: -6.69128 LUMO: 2.08711 factor:1 | 1 (-0.06286) | -1 | -1 |
| G: -5683.64846 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.75147 HOMO: -6.65318 LUMO: 2.15514 factor:1 | 1 (-0.73732) | -1 | -1 |
| G: -5683.64846 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.53888 HOMO: -6.67495 LUMO: 1.72248 factor:1 | -1 (0.47527) | -1 | -1 |
| G: -5683.64846 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11945.91844 HOMO: -6.58243 LUMO: 1.83405 factor:1 | -1 (2.09571) | -1 | -1 |
| G: -5683.64846 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11946.35428 HOMO: -6.61237 LUMO: 1.69799 factor:1 | -1 (1.65987) | -1 | -1 |
| G: -5683.64846 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.43194 HOMO: -6.57427 LUMO: 2.29936 factor:1 | -1 (0.58221) | -1 | -1 |
| G: -5683.64846 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11946.76776 HOMO: -6.40012 LUMO: 2.35378 factor:1 | -1 (1.24639) | -1 | -1 |
| G: -5683.64846 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.84092 HOMO: -6.90081 LUMO: 2.26671 factor:1 | -1 (0.17323) | -1 | -1 |
| G: -5683.64846 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.72577 HOMO: -6.44910 LUMO: 2.25855 factor:1 | -1 (0.28839) | -1 | -1 |
| G: -5683.64846 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.51520 HOMO: -6.61509 LUMO: 2.26943 factor:1 | 1 (-0.50104) | -1 | -1 |
| G: -5683.64846 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.74023 HOMO: -6.78924 LUMO: 2.09256 factor:1 | 1 (-0.72608) | -1 | -1 |
| G: -5683.64846 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.59205 HOMO: -6.47087 LUMO: 1.97555 factor:1 | -1 (0.42210) | -1 | -1 |
| G: -5683.64846 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.13160 HOMO: -6.75931 LUMO: 1.98643 factor:1 | 1 (-0.11744) | -1 | -1 |
| G: -5683.64846 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.54124 HOMO: -6.17971 LUMO: 2.09800 factor:1 | 1 (-0.52708) | -1 | -1 |
| G: -5683.64846 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.48673 HOMO: -6.83006 LUMO: 1.91840 factor:1 | 1 (-0.47258) | -1 | -1 |
| G: -5683.64846 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.70860 HOMO: -6.72938 LUMO: 2.17419 factor:1 | 1 (-1.69445) | -1 | -1 |
| G: -5683.64846 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.12269 HOMO: -6.78924 LUMO: 2.42726 factor:1 | 1 (-1.10854) | -1 | -1 |
| G: -5683.64846 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.78812 HOMO: -6.41372 LUMO: 1.93745 factor:1 | 1 (-1.77396) | -1 | -1 |
| G: -5683.64846 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.14843 HOMO: -6.85455 LUMO: 2.14970 factor:1 | 1 (-1.13428) | -1 | -1 |
| G: -5683.64846 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.43464 HOMO: -6.38651 LUMO: 2.18507 factor:1 | 1 (-1.42049) | -1 | -1 |
| G: -5683.64846 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.66946 HOMO: -6.81373 LUMO: 2.00548 factor:1 | 1 (-0.65530) | -1 | -1 |
| G: -5683.64846 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.73629 HOMO: -6.64774 LUMO: 2.41365 factor:1 | 1 (-0.72214) | -1 | -1 |
| G: -5683.64846 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.53547 HOMO: -6.70489 LUMO: 2.31569 factor:1 | 1 (-0.52132) | -1 | -1 |
| G: -5683.64846 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.87763 HOMO: -6.49264 LUMO: 1.78779 factor:1 | -1 (0.13652) | -1 | -1 |
| G: -5683.64846 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.56848 HOMO: -6.81101 LUMO: 1.86670 factor:1 | -1 (0.44567) | -1 | -1 |
| G: -5683.64846 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.45574 HOMO: -6.72121 LUMO: 1.48846 factor:1 | 1 (-0.44159) | -1 | -1 |
| G: -5683.64846 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.41662 HOMO: -6.35930 LUMO: 1.78507 factor:1 | -1 (0.59753) | -1 | -1 |
| G: -5683.64846 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.60887 HOMO: -6.38651 LUMO: 2.04358 factor:1 | -1 (0.40529) | -1 | -1 |
| G: -5683.64846 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11946.14848 HOMO: -6.42189 LUMO: 1.99187 factor:1 | -1 (1.86567) | -1 | -1 |
| G: -5683.64846 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11946.74850 HOMO: -6.69400 LUMO: 1.61091 factor:1 | -1 (1.26566) | -1 | -1 |
| G: -5683.64846 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11945.98674 HOMO: -6.81101 LUMO: 2.17419 factor:1 | -1 (2.02741) | -1 | -1 |
| G: -5683.64846 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11946.58585 HOMO: -6.90897 LUMO: 2.28576 factor:1 | -1 (1.42830) | -1 | -1 |
| G: -5683.64846 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11946.35709 HOMO: -6.75387 LUMO: 2.31297 factor:1 | -1 (1.65706) | -1 | -1 |
| G: -5683.64846 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11946.70874 HOMO: -7.05863 LUMO: 2.18780 factor:1 | -1 (1.30541) | -1 | -1 |
| G: -5683.64846 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11946.83345 HOMO: -6.56611 LUMO: 1.99187 factor:1 | -1 (1.18070) | -1 | -1 |
| G: -5683.64846 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11946.33880 HOMO: -6.59060 LUMO: 1.86398 factor:1 | -1 (1.67535) | -1 | -1 |
| G: -5683.64846 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11946.70343 HOMO: -6.59060 LUMO: 1.59459 factor:1 | -1 (1.31072) | -1 | -1 |
| G: -5683.64846 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.70266 HOMO: -6.57699 LUMO: 1.48030 factor:1 | -1 (0.31149) | -1 | -1 |
| G: -5683.64846 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.25131 HOMO: -6.99605 LUMO: 2.30208 factor:1 | -1 (0.76284) | -1 | -1 |
| G: -5683.64846 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11946.99778 HOMO: -6.42189 LUMO: 2.20412 factor:1 | -1 (1.01637) | -1 | -1 |
| G: -5683.64846 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11946.49423 HOMO: -7.15115 LUMO: 1.83405 factor:1 | -1 (1.51992) | 1 | 1 |
| G: -5683.64846 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11946.11077 HOMO: -7.08040 LUMO: 2.21773 factor:1 | -1 (1.90338) | 1 | 1 |
| G: -5683.64846 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11946.45197 HOMO: -6.72121 LUMO: 1.89663 factor:1 | -1 (1.56218) | -1 | -1 |
| G: -5683.64846 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11946.99484 HOMO: -6.25590 LUMO: 1.85037 factor:1 | -1 (1.01931) | -1 | -1 |
| G: -5683.64846 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11946.58406 HOMO: -6.70489 LUMO: 1.98915 factor:1 | -1 (1.43009) | -1 | -1 |
| G: -5683.64846 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11946.32854 HOMO: -6.53617 LUMO: 2.08439 factor:1 | -1 (1.68561) | -1 | -1 |
| G: -5683.64846 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11945.98214 HOMO: -6.69944 LUMO: 1.98915 factor:1 | -1 (2.03201) | -1 | -1 |
| G: -5683.64846 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.52622 HOMO: -6.79468 LUMO: 1.96466 factor:1 | -1 (0.48793) | -1 | -1 |
| G: -5683.64846 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11946.62332 HOMO: -6.79468 LUMO: 1.99459 factor:1 | -1 (1.39083) | -1 | -1 |
| G: -5683.64846 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.10145 HOMO: -6.58788 LUMO: 1.98371 factor:1 | -1 (0.91270) | -1 | -1 |
| G: -5683.64846 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.52617 HOMO: -6.58788 LUMO: 2.16603 factor:1 | -1 (0.48798) | -1 | -1 |
| G: -5683.64846 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.02529 HOMO: -6.56883 LUMO: 1.64085 factor:1 | -1 (0.98886) | -1 | -1 |
| G: -5683.64846 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.50557 HOMO: -7.19197 LUMO: 2.66127 factor:1 | -1 (0.50858) | 1 | 1 |
| G: -5683.64846 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.86185 HOMO: -6.48175 LUMO: 2.40004 factor:1 | -1 (0.15230) | -1 | -1 |
| G: -5683.64846 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11946.96314 HOMO: -6.18515 LUMO: 2.27759 factor:1 | -1 (1.05101) | -1 | -1 |
| G: -5683.64846 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.60087 HOMO: -6.64774 LUMO: 2.13337 factor:1 | -1 (0.41329) | -1 | -1 |
| G: -5683.64846 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.81243 HOMO: -6.39740 LUMO: 1.95106 factor:1 | -1 (0.20172) | -1 | -1 |
| G: -5683.64846 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.16600 HOMO: -6.59332 LUMO: 1.81772 factor:1 | -1 (0.84815) | -1 | -1 |
| G: -5683.64846 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.00668 HOMO: -6.68312 LUMO: 2.41909 factor:1 | -1 (1.00747) | -1 | -1 |
| G: -5683.64846 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.52292 HOMO: -5.87494 LUMO: 2.18235 factor:1 | 1 (-0.50877) | -1 | -1 |
| G: -5683.64846 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.51672 HOMO: -6.30488 LUMO: 2.04902 factor:1 | 1 (-0.50257) | -1 | -1 |
| G: -5683.64846 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.41089 HOMO: -6.65046 LUMO: 2.05446 factor:1 | 1 (-0.39674) | -1 | -1 |
| G: -5683.64846 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.17745 HOMO: -6.55794 LUMO: 2.06807 factor:1 | 1 (-0.16330) | -1 | -1 |
| G: -5683.64846 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11946.47472 HOMO: -6.68040 LUMO: 1.99187 factor:1 | -1 (1.53943) | -1 | -1 |
| G: -5683.64846 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11946.38011 HOMO: -6.60965 LUMO: 2.18780 factor:1 | -1 (1.63404) | -1 | -1 |
| G: -5683.64846 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11946.91070 HOMO: -6.88176 LUMO: 2.10344 factor:1 | -1 (1.10345) | -1 | -1 |
| G: -5683.64846 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.09797 HOMO: -6.63414 LUMO: 1.70615 factor:1 | -1 (0.91618) | -1 | -1 |
| G: -5683.64846 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11946.99685 HOMO: -7.15115 LUMO: 2.07351 factor:1 | -1 (1.01730) | 1 | 1 |
| G: -5683.64846 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11946.98172 HOMO: -6.85727 LUMO: 2.27759 factor:1 | -1 (1.03243) | -1 | -1 |
| G: -5683.64846 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.05195 HOMO: -6.91713 LUMO: 2.28848 factor:1 | 1 (-0.03780) | -1 | -1 |
| G: -5683.64846 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11946.21306 HOMO: -7.10217 LUMO: 2.14698 factor:1 | -1 (1.80109) | 1 | 1 |
| G: -5683.64846 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11946.47157 HOMO: -6.78108 LUMO: 2.45447 factor:1 | -1 (1.54259) | -1 | -1 |
| G: -5683.64846 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.17531 HOMO: -6.78380 LUMO: 2.43542 factor:1 | -1 (0.83885) | -1 | -1 |
| G: -5683.64846 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.28268 HOMO: -6.60965 LUMO: 2.33474 factor:1 | -1 (0.73147) | -1 | -1 |
| G: -5683.64846 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.74394 HOMO: -6.72665 LUMO: 2.25855 factor:1 | -1 (0.27021) | -1 | -1 |
| G: -5683.64846 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11946.85584 HOMO: -6.27495 LUMO: 2.04358 factor:1 | -1 (1.15831) | -1 | -1 |
| G: -5683.64846 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11946.88352 HOMO: -6.17426 LUMO: 1.45853 factor:1 | -1 (1.13063) | -1 | -1 |
| G: -5683.64846 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.21335 HOMO: -7.21374 LUMO: 2.33474 factor:1 | -1 (0.80080) | 1 | 1 |
| G: -5683.64846 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.35784 HOMO: -6.94707 LUMO: 1.81772 factor:1 | -1 (0.65631) | -1 | -1 |
| G: -5683.64846 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.80577 HOMO: -6.80829 LUMO: 0.17960 factor:1 | -1 (0.20838) | -1 | -1 |
| G: -5683.64846 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.28374 HOMO: -7.19469 LUMO: 1.60819 factor:1 | -1 (0.73041) | 1 | 1 |
| G: -5683.64846 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.77883 HOMO: -6.78652 LUMO: 0.53334 factor:1 | -1 (0.23532) | -1 | -1 |
| G: -5683.64846 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.15963 HOMO: -6.70489 LUMO: 0.74559 factor:1 | -1 (0.85452) | -1 | -1 |
| G: -5683.64846 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11946.60920 HOMO: -6.72393 LUMO: 0.88981 factor:1 | -1 (1.40495) | -1 | -1 |
| G: -5683.64846 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.24551 HOMO: -4.54430 LUMO: -0.90614 factor:1 | -1 (0.76864) | -1 | -1 |
| G: -5683.64846 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11946.43445 HOMO: -6.83006 LUMO: 0.47348 factor:1 | -1 (1.57970) | -1 | -1 |
| G: -5683.64846 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11946.60915 HOMO: -7.07496 LUMO: 0.50613 factor:1 | -1 (1.40501) | -1 | -1 |
| G: -5683.64846 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11946.70994 HOMO: -6.62053 LUMO: 0.74559 factor:1 | -1 (1.30421) | -1 | -1 |
| G: -5683.64846 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.22079 HOMO: -6.79196 LUMO: 1.80139 factor:1 | 1 (-1.20663) | -1 | -1 |
| G: -5683.64846 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.78317 HOMO: -6.71033 LUMO: 0.40817 factor:1 | 1 (-0.76902) | -1 | -1 |
| G: -5683.64846 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.73468 HOMO: -6.74026 LUMO: 0.95784 factor:1 | 1 (-0.72053) | -1 | -1 |
| G: -5683.64846 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.76883 HOMO: -7.34707 LUMO: 0.40001 factor:1 | 1 (-0.75468) | -1 | -1 |
| G: -5683.64846 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.77368 HOMO: -6.19875 LUMO: -0.88709 factor:1 | 1 (-0.75952) | -1 | -1 |
| G: -5683.64846 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.70529 HOMO: -6.48719 LUMO: -0.14694 factor:1 | 1 (-1.69113) | -1 | -1 |
| G: -5683.64846 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.96652 HOMO: -6.73482 LUMO: -0.01633 factor:1 | 1 (-0.95237) | -1 | -1 |
| G: -5683.64846 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.74262 HOMO: -7.05591 LUMO: -0.20136 factor:1 | 1 (-1.72847) | -1 | -1 |
| G: -5683.64846 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.99885 HOMO: -6.38651 LUMO: -2.07895 factor:1 | 1 (-0.98470) | -1 | -1 |
| G: -5683.64846 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.44697 HOMO: -6.85455 LUMO: -1.03403 factor:1 | 1 (-1.43282) | -1 | -1 |
| G: -5683.64846 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.94885 HOMO: -6.72121 LUMO: -0.99322 factor:1 | 1 (-1.93470) | -1 | -1 |
| G: -5683.64846 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.64357 HOMO: -6.53890 LUMO: -0.10885 factor:1 | 1 (-1.62942) | -1 | -1 |
| G: -5683.64846 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.73193 HOMO: -6.68312 LUMO: 0.21225 factor:1 | 1 (-0.71778) | -1 | -1 |
| G: -5683.64846 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.16283 HOMO: -6.68040 LUMO: 0.21225 factor:1 | 1 (-1.14867) | -1 | -1 |
| G: -5683.64846 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.66127 HOMO: -6.76475 LUMO: -0.64491 factor:1 | 1 (-0.64711) | -1 | -1 |
| G: -5683.64846 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.11946 HOMO: -6.48175 LUMO: 0.41633 factor:1 | 1 (-0.10531) | -1 | -1 |
| G: -5683.64846 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.06734 HOMO: -6.42733 LUMO: 0.16599 factor:1 | 1 (-1.05319) | -1 | -1 |
| G: -5683.64846 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.81723 HOMO: -6.66679 LUMO: 0.77825 factor:1 | 1 (-1.80308) | -1 | -1 |
| G: -5683.64846 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.86678 HOMO: -6.75931 LUMO: -0.73471 factor:1 | 1 (-1.85263) | -1 | -1 |
| G: -5683.64846 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.18454 HOMO: -6.53617 LUMO: 0.38096 factor:1 | 1 (-1.17039) | -1 | -1 |
| G: -5683.64846 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.81027 HOMO: -6.34297 LUMO: 0.35375 factor:1 | 1 (-1.79611) | -1 | -1 |
| G: -5683.64846 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.23022 HOMO: -7.11850 LUMO: -0.03265 factor:1 | 1 (-2.21607) | -1 | -1 |
| G: -5683.64846 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.03110 HOMO: -5.21914 LUMO: 1.29798 factor:1 | 1 (-1.01694) | -1 | -1 |
| G: -5683.64846 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.30272 HOMO: -7.09129 LUMO: -0.66668 factor:1 | 1 (-1.28857) | -1 | -1 |
| G: -5683.64846 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.17392 HOMO: -6.96884 LUMO: -0.31021 factor:1 | 1 (-2.15977) | -1 | -1 |
| G: -5683.64846 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.57179 HOMO: -6.51713 LUMO: -0.59865 factor:1 | 1 (-0.55764) | -1 | -1 |
| G: -5683.64846 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.35241 HOMO: -6.69400 LUMO: -0.07075 factor:1 | 1 (-1.33826) | -1 | -1 |
| G: -5683.64846 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.65961 HOMO: -5.28173 LUMO: 1.17281 factor:1 | -1 (0.35454) | -1 | -1 |
| G: -5683.64846 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.54214 HOMO: -6.54434 LUMO: 0.32109 factor:1 | -1 (0.47201) | -1 | -1 |
| G: -5683.64846 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.16666 HOMO: -6.79740 LUMO: -0.24762 factor:1 | 1 (-1.15251) | -1 | -1 |
| G: -5683.64846 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.25401 HOMO: -6.91986 LUMO: -0.14694 factor:1 | 1 (-1.23986) | -1 | -1 |
| G: -5683.64846 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.77944 HOMO: -6.75114 LUMO: 0.18504 factor:1 | 1 (-0.76529) | -1 | -1 |
| G: -5683.64846 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.96339 HOMO: -6.74842 LUMO: 0.69389 factor:1 | 1 (-0.94924) | -1 | -1 |
| G: -5683.64846 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.69857 HOMO: -7.01782 LUMO: 0.56600 factor:1 | 1 (-0.68442) | -1 | -1 |
| G: -5683.64846 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.68460 HOMO: -6.47359 LUMO: -0.56600 factor:1 | 1 (-1.67045) | -1 | -1 |
| G: -5683.64846 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.96865 HOMO: -6.63686 LUMO: -0.55783 factor:1 | -1 (0.04550) | -1 | -1 |
| G: -5683.64846 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.87880 HOMO: -4.13885 LUMO: -2.05446 factor:1 | -1 (0.13535) | -1 | -1 |
| G: -5683.64846 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.75869 HOMO: -6.34570 LUMO: 0.19864 factor:1 | -1 (0.25546) | -1 | -1 |
| G: -5683.64846 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.42687 HOMO: -6.47903 LUMO: 0.24762 factor:1 | 1 (-0.41272) | -1 | -1 |
| G: -5683.64846 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.10773 HOMO: -6.15249 LUMO: 0.32109 factor:1 | 1 (-0.09358) | -1 | -1 |
| G: -5683.64846 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.69816 HOMO: -6.84366 LUMO: 0.29116 factor:1 | 1 (-0.68401) | -1 | -1 |
| G: -5683.64846 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.91858 HOMO: -6.34297 LUMO: 0.19864 factor:1 | 1 (-0.90442) | -1 | -1 |
| G: -5683.64846 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.84176 HOMO: -6.51168 LUMO: 0.30749 factor:1 | 1 (-0.82761) | -1 | -1 |
| G: -5683.64846 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.10704 HOMO: -6.79468 LUMO: -0.16599 factor:1 | 1 (-1.09289) | -1 | -1 |
| G: -5683.64846 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11946.64297 HOMO: -7.24095 LUMO: 0.15238 factor:1 | -1 (1.37118) | -1 | -1 |
| G: -5683.64846 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.59288 HOMO: -7.06952 LUMO: -0.34558 factor:1 | 1 (-0.57873) | -1 | -1 |
| G: -5683.64846 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.24200 HOMO: -6.88176 LUMO: 0.02177 factor:1 | -1 (0.77215) | -1 | -1 |
| G: -5683.64846 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.02052 HOMO: -6.37291 LUMO: -0.69117 factor:1 | 1 (-0.00637) | -1 | -1 |
| G: -5683.64846 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.05980 HOMO: -6.83278 LUMO: -0.59049 factor:1 | 1 (-1.04565) | -1 | -1 |
| G: -5683.64846 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.81571 HOMO: -6.57155 LUMO: -0.33470 factor:1 | 1 (-1.80156) | -1 | -1 |
| G: -5683.64846 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.71220 HOMO: -6.89537 LUMO: -0.58504 factor:1 | 1 (-1.69804) | -1 | -1 |
| G: -5683.64846 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.01711 HOMO: -6.57155 LUMO: -0.34831 factor:1 | 1 (-1.00296) | -1 | -1 |
| G: -5683.64846 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.56311 HOMO: -6.64774 LUMO: -0.95784 factor:1 | 1 (-0.54896) | -1 | -1 |
| G: -5683.64846 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11946.59502 HOMO: -6.91713 LUMO: -0.69933 factor:1 | -1 (1.41913) | -1 | -1 |
| G: -5683.64846 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.57892 HOMO: -6.80557 LUMO: -0.65035 factor:1 | 1 (-0.56477) | -1 | -1 |
| G: -5683.64846 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.77518 HOMO: -7.26544 LUMO: -0.79729 factor:1 | -1 (0.23897) | -1 | -1 |
| G: -5683.64846 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.67444 HOMO: -6.69128 LUMO: -0.16871 factor:1 | -1 (0.33971) | -1 | -1 |
| G: -5683.64846 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.33611 HOMO: -6.88448 LUMO: 0.13061 factor:1 | 1 (-1.32196) | -1 | -1 |
| G: -5683.64846 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.18673 HOMO: -6.50352 LUMO: 0.12245 factor:1 | 1 (-0.17257) | -1 | -1 |
| G: -5683.64846 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.80198 HOMO: -6.56067 LUMO: 0.17687 factor:1 | 1 (-0.78782) | -1 | -1 |
| G: -5683.64846 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.92550 HOMO: -6.70216 LUMO: 0.25034 factor:1 | -1 (0.08865) | -1 | -1 |
| G: -5683.64846 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.51433 HOMO: -6.51713 LUMO: -0.78369 factor:1 | -1 (0.49982) | -1 | -1 |
| G: -5683.64846 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.38362 HOMO: -6.50352 LUMO: 0.12245 factor:1 | 1 (-1.36947) | -1 | -1 |
| G: -5683.64846 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.95719 HOMO: -6.22052 LUMO: -0.83811 factor:1 | 1 (-0.94304) | -1 | -1 |
| G: -5683.64846 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.79670 HOMO: -6.51168 LUMO: -0.76464 factor:1 | 1 (-0.78255) | -1 | -1 |
| G: -5683.64846 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.41328 HOMO: -7.14571 LUMO: -0.80274 factor:1 | 1 (-1.39913) | -1 | -1 |
| G: -5683.64846 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.89825 HOMO: -6.66679 LUMO: -0.88709 factor:1 | 1 (-0.88410) | -1 | -1 |
| G: -5683.64846 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.39042 HOMO: -6.76203 LUMO: -1.43948 factor:1 | 1 (-1.37627) | -1 | -1 |
| G: -5683.64846 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.56181 HOMO: -6.57427 LUMO: -1.62996 factor:1 | 1 (-0.54766) | -1 | -1 |
| G: -5683.64846 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11946.97402 HOMO: -5.05043 LUMO: 1.24900 factor:1 | -1 (1.04013) | -1 | -1 |
| G: -5683.64846 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.08137 HOMO: -6.53345 LUMO: 0.23130 factor:1 | -1 (0.93278) | -1 | -1 |
| G: -5683.64846 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11946.98700 HOMO: -7.18381 LUMO: -0.22585 factor:1 | -1 (1.02715) | -1 | -1 |
| G: -5683.64846 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.16668 HOMO: -7.00965 LUMO: -1.79595 factor:1 | -1 (0.84747) | -1 | -1 |
| G: -5683.64846 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11946.38794 HOMO: -6.08174 LUMO: -0.82995 factor:1 | -1 (1.62621) | -1 | -1 |
| G: -5683.64846 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11946.20127 HOMO: -6.42189 LUMO: -0.84355 factor:1 | -1 (1.81288) | -1 | -1 |
| G: -5683.64846 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11946.44680 HOMO: -6.53890 LUMO: 0.60409 factor:1 | -1 (1.56735) | -1 | -1 |
| G: -5683.64846 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.74005 HOMO: -6.62869 LUMO: 0.43810 factor:1 | -1 (0.27410) | -1 | -1 |
| G: -5683.64846 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.35520 HOMO: -6.68312 LUMO: 0.64491 factor:1 | -1 (0.65895) | -1 | -1 |
| G: -5683.64846 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11946.95576 HOMO: -6.42189 LUMO: 1.51295 factor:1 | -1 (1.05839) | -1 | -1 |
| G: -5683.64846 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.94451 HOMO: -6.17971 LUMO: 1.67622 factor:1 | 1 (-0.93036) | -1 | -1 |
| G: -5683.64846 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.85341 HOMO: -6.79196 LUMO: 1.36873 factor:1 | 1 (-0.83925) | -1 | -1 |
| G: -5683.64846 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.88247 HOMO: -7.38517 LUMO: 0.56328 factor:1 | 1 (-0.86832) | 1 | 1 |
| G: -5683.64846 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.33347 HOMO: -7.56204 LUMO: 0.71566 factor:1 | 1 (-1.31932) | 1 | 1 |
| G: -5683.64846 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.99939 HOMO: -6.45726 LUMO: -1.91840 factor:1 | 1 (-0.98524) | -1 | -1 |
| G: -5683.64846 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.62481 HOMO: -6.13073 LUMO: -0.97417 factor:1 | -1 (0.38934) | -1 | -1 |
| G: -5683.64846 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.28353 HOMO: -6.50352 LUMO: -0.69661 factor:1 | -1 (0.73063) | -1 | -1 |
| G: -5683.64846 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.18428 HOMO: -6.76747 LUMO: -1.71976 factor:1 | 1 (-0.17013) | -1 | -1 |
| G: -5683.64846 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11946.61048 HOMO: -6.48447 LUMO: -0.89525 factor:1 | -1 (1.40367) | -1 | -1 |
| G: -5683.64846 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.17512 HOMO: -7.11850 LUMO: -0.71566 factor:1 | -1 (0.83904) | -1 | -1 |
| G: -5683.64846 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.59133 HOMO: -6.80285 LUMO: -0.49253 factor:1 | 1 (-0.57718) | -1 | -1 |
| G: -5683.64846 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.48480 HOMO: -6.80557 LUMO: -0.88165 factor:1 | 1 (-0.47065) | -1 | -1 |
| G: -5683.64846 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11946.20147 HOMO: -6.94162 LUMO: -0.08980 factor:1 | -1 (1.81269) | -1 | -1 |
| G: -5683.64846 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11946.10149 HOMO: -6.97972 LUMO: -0.29388 factor:1 | -1 (1.91266) | -1 | -1 |
| G: -5683.64846 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.23022 HOMO: -6.75114 LUMO: 0.04626 factor:1 | -1 (0.78393) | -1 | -1 |
| G: -5683.64846 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11946.76888 HOMO: -7.15932 LUMO: 0.68845 factor:1 | -1 (1.24527) | 1 | 1 |
| G: -5683.64846 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.38453 HOMO: -7.36612 LUMO: 0.63675 factor:1 | 1 (-0.37037) | 1 | 1 |
| G: -5683.64846 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.52448 HOMO: -7.02598 LUMO: -0.66124 factor:1 | -1 (0.48967) | -1 | -1 |
| G: -5683.64846 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.25750 HOMO: -6.89264 LUMO: -0.54967 factor:1 | 1 (-0.24335) | -1 | -1 |
| G: -5683.64846 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.47934 HOMO: -6.97700 LUMO: 0.27756 factor:1 | -1 (0.53481) | -1 | -1 |
| G: -5683.64846 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11946.23521 HOMO: -6.60965 LUMO: 0.08163 factor:1 | -1 (1.77894) | -1 | -1 |
| G: -5683.64846 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11946.23344 HOMO: -6.70761 LUMO: 0.40001 factor:1 | -1 (1.78071) | -1 | -1 |
| G: -5683.64846 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11946.09880 HOMO: -6.69128 LUMO: 0.23674 factor:1 | -1 (1.91536) | -1 | -1 |
| G: -5683.64846 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.64276 HOMO: -6.69128 LUMO: -0.69933 factor:1 | 1 (-0.62861) | -1 | -1 |
| G: -5683.64846 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.07012 HOMO: -6.18515 LUMO: -0.85988 factor:1 | 1 (-1.05597) | -1 | -1 |
| G: -5683.64846 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.15674 HOMO: -6.86815 LUMO: -1.90208 factor:1 | 1 (-0.14259) | -1 | -1 |
| G: -5683.64846 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.56169 HOMO: -6.37563 LUMO: -1.74697 factor:1 | 1 (-1.54754) | -1 | -1 |
| G: -5683.64846 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.82832 HOMO: -6.75659 LUMO: 0.36463 factor:1 | 1 (-0.81416) | -1 | -1 |
| G: -5683.64846 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.27017 HOMO: -6.91441 LUMO: -0.88981 factor:1 | 1 (-1.25602) | -1 | -1 |
| G: -5683.64846 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.04035 HOMO: -6.71305 LUMO: -0.29933 factor:1 | 1 (-1.02620) | -1 | -1 |
| G: -5683.64846 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.95224 HOMO: -6.91441 LUMO: -1.04492 factor:1 | 1 (-0.93809) | -1 | -1 |
| G: -5683.64846 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.75291 HOMO: -6.05453 LUMO: -0.83539 factor:1 | 1 (-0.73876) | -1 | -1 |
| G: -5683.64846 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.72520 HOMO: -7.35252 LUMO: -0.45715 factor:1 | 1 (-1.71105) | -1 | -1 |
| G: -5683.64846 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.92015 HOMO: -6.41644 LUMO: -0.97417 factor:1 | 1 (-0.90600) | -1 | -1 |
| G: -5683.64846 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.05437 HOMO: -6.78924 LUMO: 0.36735 factor:1 | 1 (-0.04022) | -1 | -1 |
| G: -5683.64846 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.97882 HOMO: -6.74298 LUMO: 0.51974 factor:1 | 1 (-0.96467) | -1 | -1 |
| G: -5683.64846 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.00774 HOMO: -6.48992 LUMO: 1.44765 factor:1 | -1 (1.00641) | -1 | -1 |
| G: -5683.64846 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.02243 HOMO: -6.12528 LUMO: 1.57826 factor:1 | -1 (0.99172) | -1 | -1 |
| G: -5683.64846 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.39901 HOMO: -6.62325 LUMO: 1.57826 factor:1 | -1 (0.61514) | -1 | -1 |
| G: -5683.64846 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.87630 HOMO: -6.19875 LUMO: 1.29798 factor:1 | -1 (0.13785) | -1 | -1 |
| G: -5683.64846 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.32595 HOMO: -6.74570 LUMO: 1.52112 factor:1 | -1 (0.68820) | -1 | -1 |
| G: -5683.64846 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11946.71652 HOMO: -6.84094 LUMO: 1.48574 factor:1 | -1 (1.29763) | -1 | -1 |
| G: -5683.64846 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11946.97517 HOMO: -6.85183 LUMO: 0.33470 factor:1 | -1 (1.03899) | -1 | -1 |
| G: -5683.64846 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.06058 HOMO: -6.51168 LUMO: 0.48164 factor:1 | -1 (0.95357) | -1 | -1 |
| G: -5683.64846 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11946.73475 HOMO: -6.25046 LUMO: 0.75648 factor:1 | -1 (1.27940) | -1 | -1 |
| G: -5683.64846 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11946.39663 HOMO: -6.65591 LUMO: 0.32109 factor:1 | -1 (1.61753) | -1 | -1 |
| G: -5683.64846 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11946.10759 HOMO: -6.71033 LUMO: 0.40817 factor:1 | -1 (1.90657) | -1 | -1 |
| G: -5683.64846 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.35164 HOMO: -6.75114 LUMO: 0.73471 factor:1 | -1 (0.66252) | -1 | -1 |
| G: -5683.64846 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.86656 HOMO: -6.50624 LUMO: 0.59321 factor:1 | -1 (0.14759) | -1 | -1 |
| G: -5683.64846 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11946.84627 HOMO: -6.39740 LUMO: 0.83267 factor:1 | -1 (1.16789) | -1 | -1 |
| G: -5683.64846 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11946.70104 HOMO: -6.44094 LUMO: 0.65579 factor:1 | -1 (1.31311) | -1 | -1 |
| G: -5683.64846 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.99646 HOMO: -6.52257 LUMO: 0.05714 factor:1 | -1 (0.01769) | -1 | -1 |
| G: -5683.64846 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11946.63685 HOMO: -7.10217 LUMO: 0.49797 factor:1 | -1 (1.37730) | -1 | -1 |
| G: -5683.64846 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.37234 HOMO: -6.83006 LUMO: 0.55783 factor:1 | 1 (-0.35818) | -1 | -1 |
| G: -5683.64846 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11946.16745 HOMO: -6.99333 LUMO: -0.79457 factor:1 | -1 (1.84670) | -1 | -1 |
| G: -5683.64846 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11945.87836 HOMO: -6.64230 LUMO: 0.32382 factor:1 | -1 (2.13579) | -1 | -1 |
| G: -5683.64846 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11945.75553 HOMO: -6.90897 LUMO: 0.30749 factor:1 | -1 (2.25863) | -1 | -1 |
| G: -5683.64846 HOMO: -7.26544 LUMO: -1.10478 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.71600 HOMO: -7.09129 LUMO: 1.33336 factor:1 | -1 (0.29816) | 1 | 1 |
| G: -5683.64846 HOMO: -7.26544 LUMO: -1.10478 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11946.94464 HOMO: -6.66951 LUMO: 1.34424 factor:1 | -1 (1.06952) | -1 | -1 |
| G: -5683.64846 HOMO: -7.26544 LUMO: -1.10478 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.18211 HOMO: -7.02870 LUMO: 1.48574 factor:1 | -1 (0.83204) | -1 | -1 |
| G: -5683.64846 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.09508 HOMO: -7.26544 LUMO: 0.32926 factor:1 | 1 (-0.08093) | -1 | -1 |
| G: -5683.64846 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.31803 HOMO: -6.56067 LUMO: -0.45987 factor:1 | -1 (0.69612) | -1 | -1 |
| G: -5683.64846 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11946.74118 HOMO: -6.54434 LUMO: -0.28300 factor:1 | -1 (1.27298) | -1 | -1 |
| G: -5683.64846 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.06538 HOMO: -7.19469 LUMO: 0.54695 factor:1 | 1 (-1.05123) | -1 | -1 |
| G: -5683.64846 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.59833 HOMO: -6.47359 LUMO: -0.22041 factor:1 | 1 (-0.58417) | -1 | -1 |
| G: -5683.64846 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.01937 HOMO: -6.80013 LUMO: 2.08167 factor:1 | 1 (-1.00522) | -1 | -1 |
| G: -5683.64846 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.92129 HOMO: -6.23957 LUMO: 1.67894 factor:1 | 1 (-1.90714) | -1 | -1 |
| G: -5683.64846 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.09284 HOMO: -6.75114 LUMO: -0.62858 factor:1 | 1 (-1.07869) | -1 | -1 |
| G: -5683.64846 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.66523 HOMO: -6.79468 LUMO: -0.64491 factor:1 | 1 (-1.65108) | -1 | -1 |
| G: -5683.64846 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.92669 HOMO: -6.84911 LUMO: -0.69661 factor:1 | 1 (-0.91253) | -1 | -1 |
| G: -5683.64846 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.65710 HOMO: -7.54028 LUMO: 0.25851 factor:1 | 1 (-0.64295) | -1 | -1 |
| G: -5683.64846 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.09607 HOMO: -6.92802 LUMO: -0.71022 factor:1 | -1 (0.91808) | -1 | -1 |
| G: -5683.64846 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.10028 HOMO: -6.72665 LUMO: -0.46804 factor:1 | -1 (0.91387) | -1 | -1 |
| G: -5683.64846 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.05724 HOMO: -6.63686 LUMO: -0.23674 factor:1 | -1 (0.95692) | -1 | -1 |
| G: -5683.64846 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.01347 HOMO: -7.21102 LUMO: 0.54423 factor:1 | -1 (0.00068) | -1 | -1 |
| G: -5683.64846 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.49169 HOMO: -6.63414 LUMO: -0.25034 factor:1 | -1 (0.52246) | -1 | -1 |
| G: -5683.64846 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.20231 HOMO: -6.70761 LUMO: -0.31837 factor:1 | 1 (-1.18816) | -1 | -1 |
| G: -5683.64846 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.76929 HOMO: -6.57155 LUMO: 1.76874 factor:1 | 1 (-1.75513) | -1 | -1 |
| G: -5683.64846 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.21777 HOMO: -6.84366 LUMO: 2.04358 factor:1 | 1 (-1.20361) | -1 | -1 |
| G: -5683.64846 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.89846 HOMO: -6.60420 LUMO: 1.80139 factor:1 | 1 (-1.88431) | -1 | -1 |
| G: -5683.64846 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.12235 HOMO: -7.03686 LUMO: 2.21229 factor:1 | 1 (-2.10820) | -1 | -1 |
| G: -5683.64846 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.71451 HOMO: -6.77564 LUMO: 1.97555 factor:1 | 1 (-1.70036) | -1 | -1 |
| G: -5683.64846 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.03306 HOMO: -6.40012 LUMO: 2.17691 factor:1 | 1 (-0.01891) | -1 | -1 |
| G: -5683.64846 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.17864 HOMO: -6.80013 LUMO: 2.25582 factor:1 | 1 (-0.16449) | -1 | -1 |
| G: -5683.64846 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.18450 HOMO: -6.74298 LUMO: 2.31569 factor:1 | 1 (-0.17034) | -1 | -1 |
| G: -5683.64846 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.83939 HOMO: -6.68856 LUMO: 1.85854 factor:1 | 1 (-0.82524) | -1 | -1 |
| G: -5683.64846 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.15619 HOMO: -6.17971 LUMO: 1.52928 factor:1 | 1 (-1.14203) | -1 | -1 |
| G: -5683.64846 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.99975 HOMO: -6.54162 LUMO: 1.91840 factor:1 | 1 (-0.98560) | -1 | -1 |
| G: -5683.64846 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.14454 HOMO: -6.80013 LUMO: -0.55511 factor:1 | 1 (-1.13039) | -1 | -1 |
| G: -5683.64846 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.95738 HOMO: -7.46953 LUMO: 0.28572 factor:1 | 1 (-0.94323) | -1 | -1 |
| G: -5683.64846 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.63813 HOMO: -6.61781 LUMO: -0.54967 factor:1 | 1 (-1.62398) | -1 | -1 |
| G: -5683.64846 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.05278 HOMO: -6.56339 LUMO: -0.47892 factor:1 | 1 (-1.03863) | -1 | -1 |
| G: -5683.64846 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.86473 HOMO: -6.65591 LUMO: -0.25307 factor:1 | 1 (-0.85057) | -1 | -1 |
| G: -5683.64846 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.70074 HOMO: -6.62869 LUMO: -0.23402 factor:1 | 1 (-1.68659) | -1 | -1 |
| G: -5683.64846 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.84816 HOMO: -6.58243 LUMO: -0.19048 factor:1 | -1 (0.16599) | -1 | -1 |
| G: -5683.64846 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.98207 HOMO: -7.27632 LUMO: 0.52790 factor:1 | -1 (0.03208) | -1 | -1 |
| G: -5683.64846 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.95257 HOMO: -7.21102 LUMO: 0.57688 factor:1 | -1 (0.06158) | -1 | -1 |
| G: -5683.64846 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.01162 HOMO: -6.72393 LUMO: -0.53879 factor:1 | -1 (0.00253) | -1 | -1 |
| G: -5683.64846 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11946.80145 HOMO: -7.42054 LUMO: -0.99322 factor:1 | -1 (1.21270) | -1 | -1 |
| G: -5683.64846 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.05871 HOMO: -6.88992 LUMO: -0.71838 factor:1 | -1 (0.95545) | -1 | -1 |
| G: -5683.64846 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11946.84899 HOMO: -6.88176 LUMO: -0.61226 factor:1 | -1 (1.16516) | -1 | -1 |
| G: -5683.64846 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.11407 HOMO: -7.36340 LUMO: -1.04492 factor:1 | 1 (-0.09992) | -1 | -1 |
| G: -5683.64846 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.15924 HOMO: -6.65863 LUMO: -0.41906 factor:1 | 1 (-0.14509) | -1 | -1 |
| G: -5683.64846 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.81762 HOMO: -7.15115 LUMO: -0.66396 factor:1 | 1 (-0.80347) | -1 | -1 |
| G: -5683.64846 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.55213 HOMO: -7.10489 LUMO: -0.64491 factor:1 | -1 (0.46202) | -1 | -1 |
| G: -5683.64846 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.06465 HOMO: -7.20285 LUMO: 0.47892 factor:1 | 1 (-1.05050) | -1 | -1 |
| G: -5683.64846 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.08715 HOMO: -6.55794 LUMO: -0.28844 factor:1 | 1 (-1.07300) | -1 | -1 |
| G: -5683.64846 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11946.64868 HOMO: -7.19197 LUMO: -0.69661 factor:1 | -1 (1.36547) | -1 | -1 |
| G: -5683.64846 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11946.84235 HOMO: -6.56883 LUMO: -0.32926 factor:1 | -1 (1.17180) | -1 | -1 |
| G: -5683.64846 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11946.81650 HOMO: -6.70761 LUMO: 1.95650 factor:1 | -1 (1.19765) | -1 | -1 |
| G: -5683.64846 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11946.58819 HOMO: -6.60420 LUMO: 1.80684 factor:1 | -1 (1.42596) | -1 | -1 |
| G: -5683.64846 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.32866 HOMO: -6.84094 LUMO: 1.64085 factor:1 | 1 (-0.31451) | -1 | -1 |
| G: -5683.64846 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.29361 HOMO: -6.69128 LUMO: 1.90208 factor:1 | 1 (-0.27946) | -1 | -1 |
| G: -5683.64846 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.71830 HOMO: -6.75387 LUMO: 1.70343 factor:1 | 1 (-0.70415) | -1 | -1 |
| G: -5683.64846 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.74775 HOMO: -7.07496 LUMO: 2.10072 factor:1 | -1 (0.26640) | -1 | -1 |
| G: -5683.64846 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.84614 HOMO: -6.99877 LUMO: 2.24494 factor:1 | 1 (-0.83199) | -1 | -1 |
| G: -5683.64846 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.97423 HOMO: -6.63414 LUMO: 2.17691 factor:1 | -1 (0.03992) | -1 | -1 |
| G: -5683.64846 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.69635 HOMO: -6.44638 LUMO: 1.78235 factor:1 | -1 (0.31780) | -1 | -1 |
| G: -5683.64846 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.86215 HOMO: -6.87632 LUMO: 1.84221 factor:1 | -1 (0.15200) | -1 | -1 |
| G: -5683.64846 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.74155 HOMO: -6.85183 LUMO: 1.68711 factor:1 | -1 (0.27260) | -1 | -1 |
| G: -5683.64846 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.80079 HOMO: -6.96339 LUMO: 2.26671 factor:1 | -1 (0.21336) | -1 | -1 |
| G: -5683.64846 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.71352 HOMO: -6.63141 LUMO: 1.96738 factor:1 | -1 (0.30063) | -1 | -1 |
| G: -5683.64846 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.75390 HOMO: -6.37019 LUMO: 2.23133 factor:1 | -1 (0.26025) | -1 | -1 |
| G: -5683.64846 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.81298 HOMO: -7.11034 LUMO: 2.32385 factor:1 | -1 (0.20117) | 1 | 1 |
| G: -5683.64846 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.39844 HOMO: -6.91986 LUMO: 1.65445 factor:1 | -1 (0.61571) | -1 | -1 |
| G: -5683.64846 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.75504 HOMO: -7.12938 LUMO: 2.28304 factor:1 | -1 (0.25911) | 1 | 1 |
| G: -5683.64846 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.68759 HOMO: -6.54978 LUMO: 1.92112 factor:1 | -1 (0.32656) | -1 | -1 |
| G: -5683.64846 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.52541 HOMO: -6.83006 LUMO: 2.48712 factor:1 | -1 (0.48874) | -1 | -1 |
| G: -5683.64846 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.76498 HOMO: -6.97972 LUMO: 1.96738 factor:1 | -1 (0.24917) | -1 | -1 |
| G: -5683.64846 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.67493 HOMO: -6.69944 LUMO: 2.06262 factor:1 | -1 (0.33922) | -1 | -1 |
| G: -5683.64846 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.54516 HOMO: -6.76747 LUMO: 2.10888 factor:1 | -1 (0.46899) | -1 | -1 |
| G: -5683.64846 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.85472 HOMO: -6.91169 LUMO: 2.06534 factor:1 | -1 (0.15943) | -1 | -1 |
| G: -5683.64846 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.86751 HOMO: -7.03414 LUMO: 1.93473 factor:1 | -1 (0.14664) | -1 | -1 |
| G: -5683.64846 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.47127 HOMO: -7.03142 LUMO: 2.52250 factor:1 | 1 (-1.45712) | -1 | -1 |
| G: -5683.64846 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.35851 HOMO: -6.34025 LUMO: 2.61229 factor:1 | 1 (-0.34436) | -1 | -1 |
| G: -5683.64846 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.72856 HOMO: -6.98788 LUMO: 2.28304 factor:1 | 1 (-0.71441) | -1 | -1 |
| G: -5683.64846 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.91842 HOMO: -6.97700 LUMO: 2.53882 factor:1 | -1 (0.09573) | -1 | -1 |
| G: -5683.64846 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.47251 HOMO: -6.58788 LUMO: 1.94289 factor:1 | -1 (0.54164) | -1 | -1 |
| G: -5683.64846 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.32566 HOMO: -6.78652 LUMO: 2.13609 factor:1 | 1 (-1.31151) | -1 | -1 |
| G: -5683.64846 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.83315 HOMO: -6.55250 LUMO: 1.82861 factor:1 | 1 (-1.81900) | -1 | -1 |
| G: -5683.64846 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.82102 HOMO: -6.45998 LUMO: 1.75786 factor:1 | 1 (-0.80687) | -1 | -1 |
| G: -5683.64846 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.30307 HOMO: -6.78924 LUMO: 2.33746 factor:1 | 1 (-1.28892) | -1 | -1 |
| G: -5683.64846 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.80918 HOMO: -6.85727 LUMO: 1.76058 factor:1 | 1 (-1.79503) | -1 | -1 |
| G: -5683.64846 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.19442 HOMO: -6.70489 LUMO: 1.84493 factor:1 | 1 (-1.18027) | -1 | -1 |
| G: -5683.64846 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.56327 HOMO: -6.71305 LUMO: 1.53472 factor:1 | 1 (-1.54912) | -1 | -1 |
| G: -5683.64846 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.05017 HOMO: -6.76747 LUMO: 1.48846 factor:1 | 1 (-1.03602) | -1 | -1 |
| G: -5683.64846 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.84056 HOMO: -6.69128 LUMO: 1.95922 factor:1 | 1 (-0.82641) | -1 | -1 |
| G: -5683.64846 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.76470 HOMO: -6.67495 LUMO: 2.05446 factor:1 | 1 (-0.75054) | -1 | -1 |
| G: -5683.64846 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.12035 HOMO: -6.63686 LUMO: 2.25310 factor:1 | 1 (-1.10620) | -1 | -1 |
| G: -5683.64846 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11946.55527 HOMO: -6.63958 LUMO: 2.14154 factor:1 | -1 (1.45888) | -1 | -1 |
| G: -5683.64846 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.33428 HOMO: -6.62597 LUMO: 2.01908 factor:1 | -1 (0.67988) | -1 | -1 |
| G: -5683.64846 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.40051 HOMO: -7.07768 LUMO: 2.14154 factor:1 | -1 (0.61364) | -1 | -1 |
| G: -5683.64846 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.30848 HOMO: -6.19603 LUMO: 2.01092 factor:1 | -1 (0.70567) | -1 | -1 |
| G: -5683.64846 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.02828 HOMO: -6.65046 LUMO: 2.15786 factor:1 | -1 (0.98587) | -1 | -1 |
| G: -5683.64846 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11946.79315 HOMO: -6.92258 LUMO: 2.31841 factor:1 | -1 (1.22100) | -1 | -1 |
| G: -5683.64846 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.01503 HOMO: -6.90081 LUMO: 2.19324 factor:1 | -1 (0.99912) | -1 | -1 |
| G: -5683.64846 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11946.93536 HOMO: -6.85455 LUMO: 1.95650 factor:1 | -1 (1.07880) | -1 | -1 |
| G: -5683.64846 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11946.57119 HOMO: -6.57699 LUMO: 1.76058 factor:1 | -1 (1.44297) | -1 | -1 |
| G: -5683.64846 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.46848 HOMO: -6.90625 LUMO: 1.97555 factor:1 | -1 (0.54567) | -1 | -1 |
| G: -5683.64846 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.43901 HOMO: -6.97428 LUMO: 1.92929 factor:1 | -1 (0.57514) | -1 | -1 |
| G: -5683.64846 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.28562 HOMO: -6.61781 LUMO: -0.41906 factor:1 | -1 (0.72853) | -1 | -1 |
| G: -5683.64846 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11946.68352 HOMO: -6.62869 LUMO: -0.81906 factor:1 | -1 (1.33064) | -1 | -1 |
| G: -5683.64846 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.01794 HOMO: -7.01237 LUMO: 2.00548 factor:1 | -1 (0.99621) | -1 | -1 |
| G: -5683.64846 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.08374 HOMO: -6.85727 LUMO: 2.17691 factor:1 | -1 (0.93041) | -1 | -1 |
| G: -5683.64846 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.75994 HOMO: -6.71849 LUMO: 1.58914 factor:1 | -1 (0.25421) | -1 | -1 |
| G: -5683.64846 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.36377 HOMO: -7.52395 LUMO: 0.27211 factor:1 | -1 (0.65038) | -1 | -1 |
| G: -5683.64846 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.32347 HOMO: -6.96611 LUMO: -0.72654 factor:1 | -1 (0.69068) | -1 | -1 |
| G: -5683.64846 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.92424 HOMO: -6.89537 LUMO: -0.68028 factor:1 | 1 (-0.91008) | -1 | -1 |
| G: -5683.64846 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.60532 HOMO: -6.84911 LUMO: -0.58504 factor:1 | 1 (-0.59117) | -1 | -1 |
| G: -5683.64846 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.64260 HOMO: -6.79196 LUMO: -0.55783 factor:1 | 1 (-0.62845) | -1 | -1 |
| G: -5683.64846 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.71629 HOMO: -6.67767 LUMO: 1.79323 factor:1 | 1 (-0.70214) | -1 | -1 |
| G: -5683.64846 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.82573 HOMO: -6.54434 LUMO: 1.91024 factor:1 | 1 (-0.81158) | -1 | -1 |
| G: -5683.64846 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.73427 HOMO: -6.62869 LUMO: 1.69799 factor:1 | 1 (-0.72012) | -1 | -1 |
| G: -5683.64846 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.85321 HOMO: -6.72393 LUMO: 2.12249 factor:1 | 1 (-1.83905) | -1 | -1 |
| G: -5683.64846 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.16353 HOMO: -6.66407 LUMO: 2.05990 factor:1 | 1 (-1.14938) | -1 | -1 |
| G: -5683.64846 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.00767 HOMO: -7.00149 LUMO: 1.82044 factor:1 | 1 (-0.99351) | -1 | -1 |
| G: -5683.64846 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.89092 HOMO: -7.12122 LUMO: 2.16058 factor:1 | 1 (-1.87677) | 1 | 1 |
| G: -5683.64846 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.20386 HOMO: -6.63141 LUMO: 2.21229 factor:1 | 1 (-1.18971) | -1 | -1 |
| G: -5683.64846 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.83775 HOMO: -6.37835 LUMO: 2.32113 factor:1 | 1 (-1.82360) | -1 | -1 |
| G: -5683.64846 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.91101 HOMO: -6.99605 LUMO: 2.00548 factor:1 | 1 (-0.89686) | -1 | -1 |
| G: -5683.64846 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.48841 HOMO: -6.85999 LUMO: 2.39460 factor:1 | 1 (-1.47426) | -1 | -1 |
| G: -5683.64846 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.92357 HOMO: -6.85727 LUMO: 2.48712 factor:1 | 1 (-1.90942) | -1 | -1 |
| G: -5683.64846 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.95074 HOMO: -7.04231 LUMO: 2.40277 factor:1 | 1 (-0.93659) | -1 | -1 |
| G: -5683.64846 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.15801 HOMO: -6.60692 LUMO: 2.26671 factor:1 | 1 (-1.14386) | -1 | -1 |
| G: -5683.64846 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.92681 HOMO: -6.67495 LUMO: 2.14698 factor:1 | 1 (-1.91266) | -1 | -1 |
| G: -5683.64846 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.47992 HOMO: -6.73210 LUMO: 2.06807 factor:1 | 1 (-1.46577) | -1 | -1 |
| G: -5683.64846 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.28852 HOMO: -7.20013 LUMO: 2.02181 factor:1 | 1 (-1.27436) | 1 | 1 |
| G: -5683.64846 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.64932 HOMO: -7.18653 LUMO: 2.29936 factor:1 | 1 (-0.63517) | 1 | 1 |
| G: -5683.64846 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.13643 HOMO: -6.92802 LUMO: 2.36195 factor:1 | 1 (-1.12228) | -1 | -1 |
| G: -5683.64846 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.92263 HOMO: -6.89537 LUMO: 1.78779 factor:1 | 1 (-0.90848) | -1 | -1 |
| G: -5683.64846 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.88864 HOMO: -6.96067 LUMO: 2.31297 factor:1 | 1 (-0.87449) | -1 | -1 |
| G: -5683.64846 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.71688 HOMO: -6.91441 LUMO: 2.50345 factor:1 | 1 (-1.70273) | -1 | -1 |
| G: -5683.64846 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.62784 HOMO: -7.17292 LUMO: 2.12521 factor:1 | 1 (-1.61369) | 1 | 1 |
| G: -5683.64846 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.82331 HOMO: -6.93618 LUMO: 2.35106 factor:1 | 1 (-0.80916) | -1 | -1 |
| G: -5683.64846 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.92941 HOMO: -6.75931 LUMO: 1.61908 factor:1 | 1 (-0.91525) | -1 | -1 |
| G: -5683.64846 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.87968 HOMO: -6.35930 LUMO: 1.23540 factor:1 | 1 (-1.86553) | -1 | -1 |
| G: -5683.64846 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.51725 HOMO: -6.17971 LUMO: 1.84493 factor:1 | 1 (-1.50310) | -1 | -1 |
| G: -5683.64846 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.17029 HOMO: -6.72665 LUMO: 2.61229 factor:1 | 1 (-0.15614) | -1 | -1 |
| G: -5683.64846 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.33439 HOMO: -6.62869 LUMO: 2.28304 factor:1 | 1 (-1.32024) | -1 | -1 |
| G: -5683.64846 HOMO: -8.88180 LUMO: 1.02315 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.03700 HOMO: -6.58243 LUMO: 0.28028 factor:1 | 1 (-1.02285) | -1 | -1 |
| G: -5683.64846 HOMO: -8.88180 LUMO: 1.02315 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.98846 HOMO: -6.79468 LUMO: 0.14966 factor:1 | 1 (-0.97430) | -1 | -1 |
| G: -5683.64846 HOMO: -8.88180 LUMO: 1.02315 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.30802 HOMO: -6.63141 LUMO: 0.31021 factor:1 | -1 (0.70614) | -1 | -1 |
| G: -5683.64846 HOMO: -8.88180 LUMO: 1.02315 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.83697 HOMO: -6.81101 LUMO: 0.13878 factor:1 | 1 (-0.82282) | -1 | -1 |
| G: -5683.64846 HOMO: -8.88180 LUMO: 1.02315 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.11814 HOMO: -6.72665 LUMO: 0.65579 factor:1 | 1 (-1.10399) | -1 | -1 |
| G: -5683.64846 HOMO: -8.88180 LUMO: 1.02315 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.00080 HOMO: -6.53073 LUMO: 0.91430 factor:1 | -1 (1.01335) | -1 | -1 |
| G: -5683.64846 HOMO: -8.88180 LUMO: 1.02315 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11946.72183 HOMO: -7.19197 LUMO: 1.62996 factor:1 | -1 (1.29232) | 1 | 1 |
| G: -5683.64846 HOMO: -8.88180 LUMO: 1.02315 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11946.58038 HOMO: -6.69400 LUMO: 0.84627 factor:1 | -1 (1.43377) | -1 | -1 |
| G: -5683.64846 HOMO: -8.88180 LUMO: 1.02315 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11946.38084 HOMO: -6.76475 LUMO: 0.51974 factor:1 | -1 (1.63331) | -1 | -1 |
| G: -5683.64846 HOMO: -8.88180 LUMO: 1.02315 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.40929 HOMO: -6.67767 LUMO: 0.52246 factor:1 | 1 (-0.39514) | -1 | -1 |
| G: -5683.64846 HOMO: -8.88180 LUMO: 1.02315 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.50590 HOMO: -6.73210 LUMO: 0.94424 factor:1 | -1 (0.50825) | -1 | -1 |
| G: -5683.64846 HOMO: -8.88180 LUMO: 1.02315 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.76298 HOMO: -6.97972 LUMO: 0.60409 factor:1 | 1 (-0.74883) | -1 | -1 |
| G: -5683.64846 HOMO: -8.88180 LUMO: 1.02315 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.84555 HOMO: -7.38517 LUMO: 0.73743 factor:1 | -1 (0.16860) | -1 | -1 |
| G: -5683.64846 HOMO: -8.88180 LUMO: 1.02315 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.06777 HOMO: -6.48992 LUMO: 1.08301 factor:1 | 1 (-2.05362) | -1 | -1 |
| G: -5683.64846 HOMO: -8.88180 LUMO: 1.02315 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.39010 HOMO: -7.18381 LUMO: 1.61908 factor:1 | 1 (-1.37594) | 1 | 1 |
| G: -5683.64846 HOMO: -8.88180 LUMO: 1.02315 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.95729 HOMO: -6.74842 LUMO: 0.57960 factor:1 | 1 (-1.94314) | -1 | -1 |
| G: -5683.64846 HOMO: -8.88180 LUMO: 1.02315 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.66205 HOMO: -6.67495 LUMO: 0.77280 factor:1 | 1 (-1.64789) | -1 | -1 |
| G: -5683.64846 HOMO: -8.88180 LUMO: 1.02315 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.66343 HOMO: -6.74570 LUMO: 0.77280 factor:1 | 1 (-1.64928) | -1 | -1 |
| G: -5683.64846 HOMO: -8.88180 LUMO: 1.02315 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.27444 HOMO: -6.73754 LUMO: 0.86804 factor:1 | 1 (-2.26029) | -1 | -1 |
| G: -5683.64846 HOMO: -8.88180 LUMO: 1.02315 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.00163 HOMO: -6.66135 LUMO: 0.94424 factor:1 | -1 (0.01252) | -1 | -1 |
| G: -5683.64846 HOMO: -8.88180 LUMO: 1.02315 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.82645 HOMO: -6.44638 LUMO: 1.00138 factor:1 | -1 (0.18770) | -1 | -1 |
| G: -5683.64846 HOMO: -8.88180 LUMO: 1.02315 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.22489 HOMO: -6.65591 LUMO: 1.02043 factor:1 | -1 (0.78927) | -1 | -1 |
| G: -5683.64846 HOMO: -8.88180 LUMO: 1.02315 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.96592 HOMO: -7.17564 LUMO: 0.50069 factor:1 | 1 (-0.95177) | -1 | -1 |
| G: -5683.64846 HOMO: -8.88180 LUMO: 1.02315 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.60678 HOMO: -6.59332 LUMO: 0.79457 factor:1 | 1 (-1.59263) | -1 | -1 |
| G: -5683.64846 HOMO: -8.88180 LUMO: 1.02315 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.51682 HOMO: -6.76747 LUMO: 1.73881 factor:1 | 1 (-1.50267) | -1 | -1 |
| G: -5683.64846 HOMO: -8.88180 LUMO: 1.02315 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.18400 HOMO: -7.00421 LUMO: 1.07485 factor:1 | 1 (-1.16984) | -1 | -1 |
| G: -5683.64846 HOMO: -8.88180 LUMO: 1.02315 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.02876 HOMO: -6.94979 LUMO: 1.67894 factor:1 | 1 (-1.01460) | -1 | -1 |
| G: -5683.64846 HOMO: -8.88180 LUMO: 1.02315 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11946.91938 HOMO: -6.66135 LUMO: 0.47076 factor:1 | -1 (1.09477) | -1 | -1 |
| G: -5683.64846 HOMO: -8.88180 LUMO: 1.02315 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.02719 HOMO: -6.74298 LUMO: 1.85037 factor:1 | -1 (0.98696) | -1 | -1 |
| G: -5683.64846 HOMO: -8.88180 LUMO: 1.02315 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.63678 HOMO: -6.65318 LUMO: 0.95240 factor:1 | 1 (-0.62262) | -1 | -1 |
| G: -5683.64846 HOMO: -8.88180 LUMO: 1.02315 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.58824 HOMO: -6.63958 LUMO: 0.78097 factor:1 | -1 (0.42591) | -1 | -1 |
| G: -5683.64846 HOMO: -8.88180 LUMO: 1.02315 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.63874 HOMO: -6.11712 LUMO: 0.40001 factor:1 | -1 (0.37541) | -1 | -1 |
| G: -5683.64846 HOMO: -8.88180 LUMO: 1.02315 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.86238 HOMO: -7.08312 LUMO: 0.92519 factor:1 | 1 (-1.84822) | -1 | -1 |
| G: -5683.64846 HOMO: -8.88180 LUMO: 1.02315 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.14683 HOMO: -6.96067 LUMO: 0.54695 factor:1 | 1 (-1.13267) | -1 | -1 |
| G: -5683.64846 HOMO: -8.88180 LUMO: 1.02315 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.23403 HOMO: -6.74026 LUMO: 0.60137 factor:1 | 1 (-2.21988) | -1 | -1 |
| G: -5683.64846 HOMO: -8.88180 LUMO: 1.02315 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.78640 HOMO: -6.74298 LUMO: 0.59593 factor:1 | 1 (-1.77225) | -1 | -1 |
| G: -5683.64846 HOMO: -8.88180 LUMO: 1.02315 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.78599 HOMO: -6.93074 LUMO: 0.60681 factor:1 | 1 (-1.77184) | -1 | -1 |
| G: -5683.64846 HOMO: -8.88180 LUMO: 1.02315 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.93166 HOMO: -6.41644 LUMO: 0.35919 factor:1 | 1 (-1.91750) | -1 | -1 |
| G: -5683.64846 HOMO: -8.88180 LUMO: 1.02315 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.23480 HOMO: -6.41917 LUMO: 1.73064 factor:1 | 1 (-1.22065) | -1 | -1 |
| G: -5683.64846 HOMO: -8.88180 LUMO: 1.02315 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.78834 HOMO: -4.64226 LUMO: -0.87893 factor:1 | 1 (-0.77419) | -1 | -1 |
| G: -5683.64846 HOMO: -8.88180 LUMO: 1.02315 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.35466 HOMO: -6.59604 LUMO: 0.90342 factor:1 | -1 (0.65950) | -1 | -1 |
| G: -5683.64846 HOMO: -8.88180 LUMO: 1.02315 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.16790 HOMO: -6.79468 LUMO: 0.50069 factor:1 | -1 (0.84625) | -1 | -1 |
| G: -5683.64846 HOMO: -8.88180 LUMO: 1.02315 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11946.92752 HOMO: -7.04503 LUMO: 0.52518 factor:1 | -1 (1.08663) | -1 | -1 |
| G: -5683.64846 HOMO: -8.88180 LUMO: 1.02315 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.56601 HOMO: -6.69400 LUMO: 0.54423 factor:1 | -1 (0.44814) | -1 | -1 |
| G: -5683.64846 HOMO: -8.88180 LUMO: 1.02315 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.77642 HOMO: -6.51713 LUMO: 0.95240 factor:1 | 1 (-0.76227) | -1 | -1 |
| G: -5683.64846 HOMO: -8.88180 LUMO: 1.02315 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.38314 HOMO: -6.88176 LUMO: 1.79323 factor:1 | 1 (-0.36899) | -1 | -1 |
| G: -5683.64846 HOMO: -8.88180 LUMO: 1.02315 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.37987 HOMO: -6.71849 LUMO: 0.28844 factor:1 | 1 (-0.36572) | -1 | -1 |
| G: -5683.64846 HOMO: -8.88180 LUMO: 1.02315 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.61979 HOMO: -6.94979 LUMO: 0.51974 factor:1 | 1 (-1.60564) | -1 | -1 |
| G: -5683.64846 HOMO: -8.88180 LUMO: 1.02315 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.96350 HOMO: -6.76203 LUMO: 0.94151 factor:1 | 1 (-0.94935) | -1 | -1 |
| G: -5683.64846 HOMO: -8.88180 LUMO: 1.02315 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.22498 HOMO: -6.91169 LUMO: 0.89525 factor:1 | 1 (-1.21083) | -1 | -1 |
| G: -5683.64846 HOMO: -8.88180 LUMO: 1.02315 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.93776 HOMO: -6.83006 LUMO: 0.89253 factor:1 | 1 (-0.92361) | -1 | -1 |
| G: -5683.64846 HOMO: -8.88180 LUMO: 1.02315 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.10168 HOMO: -7.08857 LUMO: 0.60409 factor:1 | 1 (-1.08753) | -1 | -1 |
| G: -5683.64846 HOMO: -8.88180 LUMO: 1.02315 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.29870 HOMO: -6.91713 LUMO: 1.76330 factor:1 | 1 (-0.28455) | -1 | -1 |
| G: -5683.64846 HOMO: -8.88180 LUMO: 1.02315 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.64577 HOMO: -6.47359 LUMO: 1.56193 factor:1 | 1 (-1.63162) | -1 | -1 |
| G: -5683.64846 HOMO: -6.91169 LUMO: -0.53879 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.89564 HOMO: -7.00149 LUMO: 1.47214 factor:1 | 1 (-0.88149) | -1 | -1 |
| G: -5683.64846 HOMO: -6.91169 LUMO: -0.53879 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.85275 HOMO: -7.03686 LUMO: 1.97283 factor:1 | 1 (-0.83860) | -1 | -1 |
| G: -5683.64846 HOMO: -6.91169 LUMO: -0.53879 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.97463 HOMO: -7.00965 LUMO: 1.64629 factor:1 | 1 (-0.96048) | -1 | -1 |
| G: -5683.64846 HOMO: -6.91169 LUMO: -0.53879 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.44518 HOMO: -7.06952 LUMO: 1.67622 factor:1 | 1 (-0.43103) | 1 | -1 |
| G: -5683.64846 HOMO: -6.91169 LUMO: -0.53879 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.38249 HOMO: -6.80557 LUMO: 1.70615 factor:1 | 1 (-0.36833) | -1 | -1 |
| G: -5683.64846 HOMO: -6.91169 LUMO: -0.53879 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.71056 HOMO: -6.80829 LUMO: 1.71704 factor:1 | 1 (-1.69641) | -1 | -1 |
| G: -5683.64846 HOMO: -6.91169 LUMO: -0.53879 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.74978 HOMO: -7.26544 LUMO: 1.89935 factor:1 | 1 (-1.73562) | 1 | -1 |
| G: -5683.64846 HOMO: -7.29809 LUMO: 2.83543 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.62986 HOMO: -7.00149 LUMO: 1.47214 factor:1 | 1 (-1.61570) | -1 | -1 |
| G: -5683.64846 HOMO: -7.29809 LUMO: 2.83543 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.52665 HOMO: -7.03686 LUMO: 1.97283 factor:1 | 1 (-0.51250) | -1 | -1 |
| G: -5683.64846 HOMO: -7.29809 LUMO: 2.83543 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.52203 HOMO: -7.00965 LUMO: 1.64629 factor:1 | 1 (-0.50787) | -1 | -1 |
| G: -5683.64846 HOMO: -7.29809 LUMO: 2.83543 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.27887 HOMO: -7.06952 LUMO: 1.67622 factor:1 | 1 (-2.26472) | -1 | -1 |
| G: -5683.64846 HOMO: -7.29809 LUMO: 2.83543 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.24750 HOMO: -6.80557 LUMO: 1.70615 factor:1 | 1 (-2.23335) | -1 | -1 |
| G: -5683.64846 HOMO: -7.29809 LUMO: 2.83543 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.00856 HOMO: -6.80829 LUMO: 1.71704 factor:1 | 1 (-1.99440) | -1 | -1 |
| G: -5683.64846 HOMO: -7.29809 LUMO: 2.83543 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.95177 HOMO: -7.26544 LUMO: 1.89935 factor:1 | 1 (-1.93761) | -1 | -1 |
| G: -5683.64846 HOMO: -7.85865 LUMO: 2.83543 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.55818 HOMO: -7.00149 LUMO: 1.75241 factor:1 | 1 (-1.54403) | -1 | -1 |
| G: -5683.64846 HOMO: -7.85865 LUMO: 2.83543 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.37289 HOMO: -6.91169 LUMO: 2.07079 factor:1 | 1 (-2.35874) | -1 | -1 |
| G: -5683.64846 HOMO: -7.85865 LUMO: 2.83543 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.14186 HOMO: -7.11034 LUMO: 1.76330 factor:1 | 1 (-2.12771) | -1 | -1 |
| G: -5683.64846 HOMO: -7.85865 LUMO: 2.83543 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.55014 HOMO: -6.87360 LUMO: 2.02725 factor:1 | 1 (-2.53599) | -1 | -1 |
| G: -5683.64846 HOMO: -7.85865 LUMO: 2.83543 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.25674 HOMO: -7.08584 LUMO: 1.82044 factor:1 | 1 (-0.24259) | -1 | -1 |
| G: -5683.64846 HOMO: -7.85865 LUMO: 2.83543 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.15142 HOMO: -6.90625 LUMO: 1.68166 factor:1 | 1 (-2.13726) | -1 | -1 |
| G: -5683.64846 HOMO: -7.85865 LUMO: 2.83543 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.18879 HOMO: -6.71577 LUMO: 1.93201 factor:1 | 1 (-0.17464) | -1 | -1 |
| G: -5683.64846 HOMO: -7.85865 LUMO: 2.83543 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.40798 HOMO: -6.99605 LUMO: 2.08439 factor:1 | 1 (-0.39383) | -1 | -1 |
| G: -5683.64846 HOMO: -7.85865 LUMO: 2.83543 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.97035 HOMO: -7.02326 LUMO: 1.97010 factor:1 | 1 (-1.95620) | -1 | -1 |
| G: -5683.64846 HOMO: -7.85865 LUMO: 2.83543 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.19040 HOMO: -6.99877 LUMO: 2.15514 factor:1 | 1 (-0.17625) | -1 | -1 |
| G: -5683.64846 HOMO: -7.85865 LUMO: 2.83543 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.47579 HOMO: -6.75387 LUMO: 1.95106 factor:1 | 1 (-0.46164) | -1 | -1 |
| G: -5683.64846 HOMO: -7.85865 LUMO: 2.83543 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.38083 HOMO: -7.10761 LUMO: 2.06262 factor:1 | 1 (-2.36668) | -1 | -1 |
| G: -5683.64846 HOMO: -7.85865 LUMO: 2.83543 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.44361 HOMO: -7.03142 LUMO: 1.91568 factor:1 | 1 (-2.42946) | -1 | -1 |
| G: -5683.64846 HOMO: -7.85865 LUMO: 2.83543 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.48345 HOMO: -6.98788 LUMO: 1.98371 factor:1 | 1 (-2.46930) | -1 | -1 |
| G: -5683.64846 HOMO: -7.85865 LUMO: 2.83543 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.84246 HOMO: -6.94707 LUMO: 1.68438 factor:1 | 1 (-1.82831) | -1 | -1 |
| G: -5683.64846 HOMO: -7.85865 LUMO: 2.83543 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.82290 HOMO: -6.88176 LUMO: 2.20684 factor:1 | 1 (-0.80875) | -1 | -1 |
| G: -5683.64846 HOMO: -7.85865 LUMO: 2.83543 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.97364 HOMO: -6.73210 LUMO: 2.18780 factor:1 | 1 (-1.95949) | -1 | -1 |
| G: -5683.64846 HOMO: -7.85865 LUMO: 2.83543 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.13378 HOMO: -6.83822 LUMO: 2.06807 factor:1 | 1 (-2.11963) | -1 | -1 |
| G: -5683.64846 HOMO: -7.85865 LUMO: 2.83543 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.25983 HOMO: -6.78924 LUMO: 2.42181 factor:1 | 1 (-2.24567) | -1 | -1 |
| G: -5683.64846 HOMO: -7.85865 LUMO: 2.83543 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.72113 HOMO: -6.94707 LUMO: 1.71704 factor:1 | 1 (-0.70698) | -1 | -1 |
| G: -5683.64846 HOMO: -7.85865 LUMO: 2.83543 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.74276 HOMO: -6.85183 LUMO: 1.78779 factor:1 | 1 (-1.72860) | -1 | -1 |
| G: -5683.64846 HOMO: -7.85865 LUMO: 2.83543 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.97933 HOMO: -6.98788 LUMO: 1.69799 factor:1 | 1 (-1.96518) | -1 | -1 |
| G: -5683.64846 HOMO: -7.85865 LUMO: 2.83543 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.09888 HOMO: -6.79468 LUMO: 2.04358 factor:1 | 1 (-1.08473) | -1 | -1 |
| G: -5683.64846 HOMO: -7.85865 LUMO: 2.83543 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.81101 HOMO: -6.90081 LUMO: 1.97283 factor:1 | 1 (-0.79686) | -1 | -1 |
| G: -5683.64846 HOMO: -7.85865 LUMO: 2.83543 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.79183 HOMO: -6.79468 LUMO: 2.00820 factor:1 | 1 (-0.77767) | -1 | -1 |
| G: -5683.64846 HOMO: -7.85865 LUMO: 2.83543 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.73547 HOMO: -7.06408 LUMO: 2.29936 factor:1 | 1 (-0.72132) | -1 | -1 |
| G: -5683.64846 HOMO: -7.85865 LUMO: 2.83543 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.56082 HOMO: -6.78924 LUMO: 2.13337 factor:1 | 1 (-1.54667) | -1 | -1 |
| G: -5683.64846 HOMO: -7.85865 LUMO: 2.83543 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.44874 HOMO: -6.79468 LUMO: 2.35106 factor:1 | 1 (-0.43459) | -1 | -1 |
| G: -5683.64846 HOMO: -7.85865 LUMO: 2.83543 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.64420 HOMO: -6.82734 LUMO: 2.16603 factor:1 | 1 (-1.63004) | -1 | -1 |
| G: -5683.64846 HOMO: -7.85865 LUMO: 2.83543 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.19588 HOMO: -6.79740 LUMO: 2.36739 factor:1 | 1 (-2.18173) | -1 | -1 |
| G: -5683.64846 HOMO: -7.85865 LUMO: 2.83543 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.69307 HOMO: -7.14027 LUMO: 2.10888 factor:1 | 1 (-1.67892) | -1 | -1 |
| G: -5683.64846 HOMO: -6.61509 LUMO: -0.23674 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.41257 HOMO: -6.96067 LUMO: 1.59731 factor:1 | 1 (-1.39842) | -1 | -1 |
| G: -5683.64846 HOMO: -6.61509 LUMO: -0.23674 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.62303 HOMO: -6.91169 LUMO: 1.37145 factor:1 | 1 (-1.60887) | -1 | -1 |
| G: -5683.64846 HOMO: -6.61509 LUMO: -0.23674 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.90630 HOMO: -6.94707 LUMO: 1.73064 factor:1 | 1 (-0.89215) | -1 | -1 |
| G: -5683.64846 HOMO: -6.61509 LUMO: -0.23674 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.92132 HOMO: -7.02326 LUMO: 1.41227 factor:1 | 1 (-0.90717) | -1 | -1 |
| G: -5683.64846 HOMO: -6.61509 LUMO: -0.23674 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.75404 HOMO: -6.72121 LUMO: 1.43132 factor:1 | 1 (-2.73989) | -1 | -1 |
| G: -5683.64846 HOMO: -6.61509 LUMO: -0.23674 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.45720 HOMO: -6.51168 LUMO: 1.72520 factor:1 | 1 (-1.44305) | -1 | -1 |
| G: -5683.64846 HOMO: -6.61509 LUMO: -0.23674 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.74939 HOMO: -6.98516 LUMO: 1.92929 factor:1 | 1 (-2.73523) | -1 | -1 |
| G: -5683.64846 HOMO: -6.61509 LUMO: -0.23674 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.11773 HOMO: -6.92802 LUMO: 2.07895 factor:1 | 1 (-2.10358) | -1 | -1 |
| G: -5683.64846 HOMO: -6.61509 LUMO: -0.23674 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.52285 HOMO: -7.02326 LUMO: 1.86398 factor:1 | 1 (-2.50870) | -1 | -1 |
| G: -5683.64846 HOMO: -6.61509 LUMO: -0.23674 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11951.03464 HOMO: -6.82462 LUMO: 1.86670 factor:1 | 1 (-3.02049) | -1 | -1 |
| G: -5683.64846 HOMO: -6.61509 LUMO: -0.23674 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.95459 HOMO: -6.83278 LUMO: 1.71160 factor:1 | 1 (-2.94044) | -1 | -1 |
| G: -5683.64846 HOMO: -6.61509 LUMO: -0.23674 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11951.73806 HOMO: -6.62869 LUMO: 1.69527 factor:1 | 1 (-3.72391) | -1 | -1 |
| G: -5683.64846 HOMO: -6.61509 LUMO: -0.23674 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11951.10988 HOMO: -6.84094 LUMO: 1.27349 factor:1 | 1 (-3.09573) | -1 | -1 |
| G: -5683.64846 HOMO: -6.61509 LUMO: -0.23674 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.39512 HOMO: -7.07768 LUMO: 1.27621 factor:1 | 1 (-2.38097) | 1 | -1 |
| G: -5683.64846 HOMO: -6.61509 LUMO: -0.23674 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.01424 HOMO: -7.06135 LUMO: 1.55105 factor:1 | 1 (-2.00009) | 1 | -1 |
| G: -5683.64846 HOMO: -6.61509 LUMO: -0.23674 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.53799 HOMO: -6.94162 LUMO: 1.64629 factor:1 | 1 (-1.52384) | -1 | -1 |
| G: -5683.64846 HOMO: -6.61509 LUMO: -0.23674 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.07160 HOMO: -7.07224 LUMO: 1.65445 factor:1 | 1 (-2.05745) | 1 | -1 |
| G: -5683.64846 HOMO: -6.61509 LUMO: -0.23674 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.55077 HOMO: -6.68584 LUMO: 1.91296 factor:1 | 1 (-2.53662) | -1 | -1 |
| G: -5683.64846 HOMO: -6.61509 LUMO: -0.23674 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.21300 HOMO: -7.09129 LUMO: 1.73609 factor:1 | 1 (-2.19884) | 1 | -1 |
| G: -5683.64846 HOMO: -6.61509 LUMO: -0.23674 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.13694 HOMO: -7.01237 LUMO: 2.01092 factor:1 | 1 (-2.12279) | -1 | -1 |
| G: -5683.64846 HOMO: -6.61509 LUMO: -0.23674 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.52158 HOMO: -6.93618 LUMO: 1.63540 factor:1 | 1 (-1.50743) | -1 | -1 |
| G: -5683.64846 HOMO: -6.61509 LUMO: -0.23674 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.99455 HOMO: -6.98516 LUMO: 1.64629 factor:1 | 1 (-0.98040) | -1 | -1 |
| G: -5683.64846 HOMO: -6.61509 LUMO: -0.23674 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.14100 HOMO: -6.80285 LUMO: 1.95106 factor:1 | 1 (-1.12685) | -1 | -1 |
| G: -5683.64846 HOMO: -6.61509 LUMO: -0.23674 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.01376 HOMO: -6.76747 LUMO: 1.88303 factor:1 | 1 (-0.99961) | -1 | -1 |
| G: -5683.64846 HOMO: -6.61509 LUMO: -0.23674 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.56932 HOMO: -6.64230 LUMO: 1.90480 factor:1 | 1 (-0.55517) | -1 | -1 |
| G: -5683.64846 HOMO: -6.61509 LUMO: -0.23674 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.43378 HOMO: -6.93618 LUMO: 2.19324 factor:1 | 1 (-0.41963) | -1 | -1 |
| G: -5683.64846 HOMO: -6.61509 LUMO: -0.23674 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.13126 HOMO: -6.95523 LUMO: 1.80684 factor:1 | 1 (-1.11711) | -1 | -1 |
| G: -5683.64846 HOMO: -6.61509 LUMO: -0.23674 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.94694 HOMO: -6.66135 LUMO: 1.72792 factor:1 | -1 (0.06721) | -1 | -1 |
| G: -5683.64846 HOMO: -6.61509 LUMO: -0.23674 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.32851 HOMO: -6.36202 LUMO: 1.89391 factor:1 | 1 (-2.31436) | -1 | -1 |
| G: -5683.64846 HOMO: -6.61509 LUMO: -0.23674 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.99478 HOMO: -7.03959 LUMO: 2.06262 factor:1 | 1 (-2.98063) | -1 | -1 |
| G: -5683.64846 HOMO: -6.61509 LUMO: -0.23674 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.38924 HOMO: -7.08584 LUMO: 2.01092 factor:1 | 1 (-2.37509) | 1 | -1 |
| G: -5683.64846 HOMO: -6.80285 LUMO: -0.55783 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.77285 HOMO: -6.96067 LUMO: 1.59731 factor:1 | 1 (-1.75870) | -1 | -1 |
| G: -5683.64846 HOMO: -6.80285 LUMO: -0.55783 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.05050 HOMO: -6.91169 LUMO: 1.37145 factor:1 | 1 (-1.03635) | -1 | -1 |
| G: -5683.64846 HOMO: -6.80285 LUMO: -0.55783 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.45111 HOMO: -6.94707 LUMO: 1.73064 factor:1 | 1 (-0.43696) | -1 | -1 |
| G: -5683.64846 HOMO: -6.80285 LUMO: -0.55783 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.05061 HOMO: -7.02326 LUMO: 1.41227 factor:1 | 1 (-1.03645) | -1 | -1 |
| G: -5683.64846 HOMO: -6.80285 LUMO: -0.55783 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.84396 HOMO: -6.72121 LUMO: 1.43132 factor:1 | 1 (-0.82981) | -1 | -1 |
| G: -5683.64846 HOMO: -6.80285 LUMO: -0.55783 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.92675 HOMO: -6.51168 LUMO: 1.72520 factor:1 | -1 (0.08740) | -1 | -1 |
| G: -5683.64846 HOMO: -6.80285 LUMO: -0.55783 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.17475 HOMO: -6.98516 LUMO: 1.92929 factor:1 | 1 (-0.16060) | -1 | -1 |
| G: -5683.64846 HOMO: -6.80285 LUMO: -0.55783 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.07630 HOMO: -6.92802 LUMO: 2.07895 factor:1 | 1 (-0.06215) | -1 | -1 |
| G: -5683.64846 HOMO: -6.80285 LUMO: -0.55783 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.07348 HOMO: -7.02326 LUMO: 1.86398 factor:1 | 1 (-2.05933) | -1 | -1 |
| G: -5683.64846 HOMO: -6.80285 LUMO: -0.55783 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.11118 HOMO: -6.82462 LUMO: 1.86670 factor:1 | 1 (-1.09703) | -1 | -1 |
| G: -5683.64846 HOMO: -6.80285 LUMO: -0.55783 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.02039 HOMO: -6.83278 LUMO: 1.71160 factor:1 | 1 (-2.00624) | -1 | -1 |
| G: -5683.64846 HOMO: -6.80285 LUMO: -0.55783 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.01378 HOMO: -6.62869 LUMO: 1.69527 factor:1 | 1 (-1.99963) | -1 | -1 |
| G: -5683.64846 HOMO: -6.80285 LUMO: -0.55783 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.42068 HOMO: -6.84094 LUMO: 1.27349 factor:1 | 1 (-1.40653) | -1 | -1 |
| G: -5683.64846 HOMO: -6.80285 LUMO: -0.55783 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.95509 HOMO: -7.07768 LUMO: 1.27621 factor:1 | 1 (-0.94094) | 1 | -1 |
| G: -5683.64846 HOMO: -6.80285 LUMO: -0.55783 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.24519 HOMO: -7.06135 LUMO: 1.55105 factor:1 | 1 (-1.23104) | 1 | -1 |
| G: -5683.64846 HOMO: -6.80285 LUMO: -0.55783 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.99258 HOMO: -6.94162 LUMO: 1.64629 factor:1 | 1 (-1.97843) | -1 | -1 |
| G: -5683.64846 HOMO: -6.80285 LUMO: -0.55783 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.95190 HOMO: -7.07224 LUMO: 1.65445 factor:1 | 1 (-1.93775) | 1 | -1 |
| G: -5683.64846 HOMO: -6.80285 LUMO: -0.55783 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.35826 HOMO: -6.68584 LUMO: 1.91296 factor:1 | 1 (-1.34411) | -1 | -1 |
| G: -5683.64846 HOMO: -6.80285 LUMO: -0.55783 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.32174 HOMO: -7.09129 LUMO: 1.73609 factor:1 | 1 (-1.30759) | 1 | -1 |
| G: -5683.64846 HOMO: -6.80285 LUMO: -0.55783 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.80921 HOMO: -7.01237 LUMO: 2.01092 factor:1 | 1 (-1.79505) | -1 | -1 |
| G: -5683.64846 HOMO: -6.80285 LUMO: -0.55783 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.95794 HOMO: -6.93618 LUMO: 1.63540 factor:1 | 1 (-1.94379) | -1 | -1 |
| G: -5683.64846 HOMO: -6.80285 LUMO: -0.55783 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.84726 HOMO: -6.98516 LUMO: 1.64629 factor:1 | 1 (-0.83310) | -1 | -1 |
| G: -5683.64846 HOMO: -6.80285 LUMO: -0.55783 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.63432 HOMO: -6.80285 LUMO: 1.95106 factor:1 | 1 (-1.62017) | -1 | -1 |
| G: -5683.64846 HOMO: -6.80285 LUMO: -0.55783 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.11899 HOMO: -6.76747 LUMO: 1.88303 factor:1 | 1 (-1.10484) | -1 | -1 |
| G: -5683.64846 HOMO: -6.80285 LUMO: -0.55783 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.79587 HOMO: -6.64230 LUMO: 1.90480 factor:1 | 1 (-1.78172) | -1 | -1 |
| G: -5683.64846 HOMO: -6.80285 LUMO: -0.55783 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.29333 HOMO: -6.93618 LUMO: 2.19324 factor:1 | 1 (-1.27918) | -1 | -1 |
| G: -5683.64846 HOMO: -6.80285 LUMO: -0.55783 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.50306 HOMO: -6.95523 LUMO: 1.80684 factor:1 | 1 (-0.48891) | -1 | -1 |
| G: -5683.64846 HOMO: -6.80285 LUMO: -0.55783 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.14805 HOMO: -6.66135 LUMO: 1.72792 factor:1 | 1 (-1.13390) | -1 | -1 |
| G: -5683.64846 HOMO: -6.80285 LUMO: -0.55783 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.24367 HOMO: -6.36202 LUMO: 1.89391 factor:1 | 1 (-1.22952) | -1 | -1 |
| G: -5683.64846 HOMO: -6.80285 LUMO: -0.55783 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.22816 HOMO: -7.03959 LUMO: 2.06262 factor:1 | 1 (-1.21401) | -1 | -1 |
| G: -5683.64846 HOMO: -6.80285 LUMO: -0.55783 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.89517 HOMO: -7.08584 LUMO: 2.01092 factor:1 | 1 (-1.88101) | 1 | -1 |
| G: -5683.64846 HOMO: -7.16476 LUMO: 2.86264 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.93323 HOMO: -6.96067 LUMO: 1.59731 factor:1 | 1 (-1.91908) | -1 | -1 |
| G: -5683.64846 HOMO: -7.16476 LUMO: 2.86264 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.24422 HOMO: -6.91169 LUMO: 1.37145 factor:1 | 1 (-1.23006) | -1 | -1 |
| G: -5683.64846 HOMO: -7.16476 LUMO: 2.86264 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.31924 HOMO: -6.94707 LUMO: 1.73064 factor:1 | 1 (-1.30509) | -1 | -1 |
| G: -5683.64846 HOMO: -7.16476 LUMO: 2.86264 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.76714 HOMO: -7.02326 LUMO: 1.41227 factor:1 | 1 (-1.75298) | -1 | -1 |
| G: -5683.64846 HOMO: -7.16476 LUMO: 2.86264 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.88216 HOMO: -6.72121 LUMO: 1.43132 factor:1 | 1 (-1.86801) | -1 | -1 |
| G: -5683.64846 HOMO: -7.16476 LUMO: 2.86264 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.63132 HOMO: -6.51168 LUMO: 1.72520 factor:1 | 1 (-1.61717) | -1 | -1 |
| G: -5683.64846 HOMO: -7.16476 LUMO: 2.86264 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.94241 HOMO: -6.98516 LUMO: 1.92929 factor:1 | 1 (-0.92826) | -1 | -1 |
| G: -5683.64846 HOMO: -7.16476 LUMO: 2.86264 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.37429 HOMO: -6.92802 LUMO: 2.07895 factor:1 | 1 (-1.36013) | -1 | -1 |
| G: -5683.64846 HOMO: -7.16476 LUMO: 2.86264 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.82931 HOMO: -7.02326 LUMO: 1.86398 factor:1 | 1 (-1.81516) | -1 | -1 |
| G: -5683.64846 HOMO: -7.16476 LUMO: 2.86264 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.60098 HOMO: -6.82462 LUMO: 1.86670 factor:1 | 1 (-1.58683) | -1 | -1 |
| G: -5683.64846 HOMO: -7.16476 LUMO: 2.86264 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.16647 HOMO: -6.83278 LUMO: 1.71160 factor:1 | 1 (-1.15232) | -1 | -1 |
| G: -5683.64846 HOMO: -7.16476 LUMO: 2.86264 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.95708 HOMO: -6.62869 LUMO: 1.69527 factor:1 | 1 (-0.94293) | -1 | -1 |
| G: -5683.64846 HOMO: -7.16476 LUMO: 2.86264 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.50691 HOMO: -6.84094 LUMO: 1.27349 factor:1 | 1 (-1.49276) | -1 | -1 |
| G: -5683.64846 HOMO: -7.16476 LUMO: 2.86264 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.93062 HOMO: -7.07768 LUMO: 1.27621 factor:1 | 1 (-1.91647) | -1 | -1 |
| G: -5683.64846 HOMO: -7.16476 LUMO: 2.86264 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.44053 HOMO: -7.06135 LUMO: 1.55105 factor:1 | 1 (-0.42638) | -1 | -1 |
| G: -5683.64846 HOMO: -7.16476 LUMO: 2.86264 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.54583 HOMO: -6.94162 LUMO: 1.64629 factor:1 | 1 (-1.53167) | -1 | -1 |
| G: -5683.64846 HOMO: -7.16476 LUMO: 2.86264 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.76011 HOMO: -7.07224 LUMO: 1.65445 factor:1 | 1 (-2.74596) | -1 | -1 |
| G: -5683.64846 HOMO: -7.16476 LUMO: 2.86264 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.29550 HOMO: -6.68584 LUMO: 1.91296 factor:1 | 1 (-2.28135) | -1 | -1 |
| G: -5683.64846 HOMO: -7.16476 LUMO: 2.86264 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.17376 HOMO: -7.09129 LUMO: 1.73609 factor:1 | 1 (-2.15960) | -1 | -1 |
| G: -5683.64846 HOMO: -7.16476 LUMO: 2.86264 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.52036 HOMO: -7.01237 LUMO: 2.01092 factor:1 | 1 (-1.50620) | -1 | -1 |
| G: -5683.64846 HOMO: -7.16476 LUMO: 2.86264 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.79755 HOMO: -6.93618 LUMO: 1.63540 factor:1 | 1 (-2.78340) | -1 | -1 |
| G: -5683.64846 HOMO: -7.16476 LUMO: 2.86264 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.28818 HOMO: -6.98516 LUMO: 1.64629 factor:1 | 1 (-2.27403) | -1 | -1 |
| G: -5683.64846 HOMO: -7.16476 LUMO: 2.86264 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11951.00876 HOMO: -6.80285 LUMO: 1.95106 factor:1 | 1 (-2.99461) | -1 | -1 |
| G: -5683.64846 HOMO: -7.16476 LUMO: 2.86264 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11951.66461 HOMO: -6.76747 LUMO: 1.88303 factor:1 | 1 (-3.65046) | -1 | -1 |
| G: -5683.64846 HOMO: -7.16476 LUMO: 2.86264 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.91590 HOMO: -6.64230 LUMO: 1.90480 factor:1 | 1 (-1.90175) | -1 | -1 |
| G: -5683.64846 HOMO: -7.16476 LUMO: 2.86264 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.53646 HOMO: -6.93618 LUMO: 2.19324 factor:1 | 1 (-2.52231) | -1 | -1 |
| G: -5683.64846 HOMO: -7.16476 LUMO: 2.86264 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.89391 HOMO: -6.95523 LUMO: 1.80684 factor:1 | 1 (-2.87975) | -1 | -1 |
| G: -5683.64846 HOMO: -7.16476 LUMO: 2.86264 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.89121 HOMO: -6.66135 LUMO: 1.72792 factor:1 | 1 (-2.87706) | -1 | -1 |
| G: -5683.64846 HOMO: -7.16476 LUMO: 2.86264 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.83710 HOMO: -6.36202 LUMO: 1.89391 factor:1 | 1 (-1.82295) | -1 | -1 |
| G: -5683.64846 HOMO: -7.16476 LUMO: 2.86264 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.19229 HOMO: -7.03959 LUMO: 2.06262 factor:1 | 1 (-2.17814) | -1 | -1 |
| G: -5683.64846 HOMO: -7.16476 LUMO: 2.86264 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.14519 HOMO: -7.08584 LUMO: 2.01092 factor:1 | 1 (-1.13104) | -1 | -1 |
| G: -5683.64846 HOMO: -6.50352 LUMO: 2.10888 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.36792 HOMO: -6.96067 LUMO: 1.59731 factor:1 | 1 (-1.35377) | 1 | 1 |
| G: -5683.64846 HOMO: -6.50352 LUMO: 2.10888 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.66733 HOMO: -6.91169 LUMO: 1.37145 factor:1 | 1 (-1.65317) | -1 | -1 |
| G: -5683.64846 HOMO: -6.50352 LUMO: 2.10888 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.17501 HOMO: -6.94707 LUMO: 1.73064 factor:1 | 1 (-2.16086) | 1 | 1 |
| G: -5683.64846 HOMO: -6.50352 LUMO: 2.10888 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.09295 HOMO: -7.02326 LUMO: 1.41227 factor:1 | 1 (-1.07880) | -1 | -1 |
| G: -5683.64846 HOMO: -6.50352 LUMO: 2.10888 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.00859 HOMO: -6.72121 LUMO: 1.43132 factor:1 | 1 (-0.99444) | -1 | -1 |
| G: -5683.64846 HOMO: -6.50352 LUMO: 2.10888 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.79859 HOMO: -6.51168 LUMO: 1.72520 factor:1 | 1 (-1.78444) | 1 | 1 |
| G: -5683.64846 HOMO: -6.50352 LUMO: 2.10888 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.88763 HOMO: -6.98516 LUMO: 1.92929 factor:1 | 1 (-1.87348) | 1 | 1 |
| G: -5683.64846 HOMO: -6.50352 LUMO: 2.10888 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.63989 HOMO: -6.92802 LUMO: 2.07895 factor:1 | 1 (-2.62574) | 1 | 1 |
| G: -5683.64846 HOMO: -6.50352 LUMO: 2.10888 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.65575 HOMO: -7.02326 LUMO: 1.86398 factor:1 | 1 (-2.64160) | 1 | 1 |
| G: -5683.64846 HOMO: -6.50352 LUMO: 2.10888 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.66895 HOMO: -6.82462 LUMO: 1.86670 factor:1 | 1 (-2.65480) | 1 | 1 |
| G: -5683.64846 HOMO: -6.50352 LUMO: 2.10888 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.00929 HOMO: -6.83278 LUMO: 1.71160 factor:1 | 1 (-1.99514) | 1 | 1 |
| G: -5683.64846 HOMO: -6.50352 LUMO: 2.10888 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.56983 HOMO: -6.62869 LUMO: 1.69527 factor:1 | 1 (-1.55567) | 1 | 1 |
| G: -5683.64846 HOMO: -6.50352 LUMO: 2.10888 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.90113 HOMO: -6.84094 LUMO: 1.27349 factor:1 | 1 (-1.88697) | -1 | -1 |
| G: -5683.64846 HOMO: -6.50352 LUMO: 2.10888 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.02167 HOMO: -7.07768 LUMO: 1.27621 factor:1 | 1 (-2.00752) | -1 | -1 |
| G: -5683.64846 HOMO: -6.50352 LUMO: 2.10888 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.96799 HOMO: -7.06135 LUMO: 1.55105 factor:1 | 1 (-0.95384) | -1 | -1 |
| G: -5683.64846 HOMO: -6.50352 LUMO: 2.10888 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.08876 HOMO: -6.94162 LUMO: 1.64629 factor:1 | 1 (-1.07460) | 1 | 1 |
| G: -5683.64846 HOMO: -6.50352 LUMO: 2.10888 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.46895 HOMO: -7.07224 LUMO: 1.65445 factor:1 | 1 (-1.45480) | 1 | 1 |
| G: -5683.64846 HOMO: -6.50352 LUMO: 2.10888 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.37848 HOMO: -6.68584 LUMO: 1.91296 factor:1 | 1 (-1.36432) | 1 | 1 |
| G: -5683.64846 HOMO: -6.50352 LUMO: 2.10888 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.10132 HOMO: -7.09129 LUMO: 1.73609 factor:1 | 1 (-2.08717) | 1 | 1 |
| G: -5683.64846 HOMO: -6.50352 LUMO: 2.10888 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.12938 HOMO: -7.01237 LUMO: 2.01092 factor:1 | 1 (-1.11523) | 1 | 1 |
| G: -5683.64846 HOMO: -6.50352 LUMO: 2.10888 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.89863 HOMO: -6.93618 LUMO: 1.63540 factor:1 | 1 (-0.88448) | 1 | 1 |
| G: -5683.64846 HOMO: -6.50352 LUMO: 2.10888 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.13395 HOMO: -6.98516 LUMO: 1.64629 factor:1 | 1 (-1.11980) | 1 | 1 |
| G: -5683.64846 HOMO: -6.50352 LUMO: 2.10888 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.69422 HOMO: -6.80285 LUMO: 1.95106 factor:1 | 1 (-0.68007) | 1 | 1 |
| G: -5683.64846 HOMO: -6.50352 LUMO: 2.10888 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.71247 HOMO: -6.76747 LUMO: 1.88303 factor:1 | 1 (-1.69832) | 1 | 1 |
| G: -5683.64846 HOMO: -6.50352 LUMO: 2.10888 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.49319 HOMO: -6.64230 LUMO: 1.90480 factor:1 | 1 (-2.47904) | 1 | 1 |
| G: -5683.64846 HOMO: -6.50352 LUMO: 2.10888 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.79733 HOMO: -6.93618 LUMO: 2.19324 factor:1 | 1 (-2.78318) | 1 | 1 |
| G: -5683.64846 HOMO: -6.50352 LUMO: 2.10888 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.11903 HOMO: -6.95523 LUMO: 1.80684 factor:1 | 1 (-2.10488) | 1 | 1 |
| G: -5683.64846 HOMO: -6.50352 LUMO: 2.10888 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.92150 HOMO: -6.66135 LUMO: 1.72792 factor:1 | 1 (-2.90735) | 1 | 1 |
| G: -5683.64846 HOMO: -6.50352 LUMO: 2.10888 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.09269 HOMO: -6.36202 LUMO: 1.89391 factor:1 | 1 (-2.07854) | -1 | -1 |
| G: -5683.64846 HOMO: -6.50352 LUMO: 2.10888 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.92748 HOMO: -7.03959 LUMO: 2.06262 factor:1 | 1 (-2.91333) | 1 | 1 |
| G: -5683.64846 HOMO: -6.50352 LUMO: 2.10888 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.96871 HOMO: -7.08584 LUMO: 2.01092 factor:1 | 1 (-2.95456) | 1 | 1 |
| G: -5683.64846 HOMO: -6.59604 LUMO: 2.33746 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.17740 HOMO: -6.96067 LUMO: 1.59731 factor:1 | 1 (-2.16325) | 1 | 1 |
| G: -5683.64846 HOMO: -6.59604 LUMO: 2.33746 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.77594 HOMO: -6.91169 LUMO: 1.37145 factor:1 | 1 (-2.76179) | -1 | -1 |
| G: -5683.64846 HOMO: -6.59604 LUMO: 2.33746 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.52155 HOMO: -6.94707 LUMO: 1.73064 factor:1 | 1 (-1.50740) | 1 | 1 |
| G: -5683.64846 HOMO: -6.59604 LUMO: 2.33746 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.11612 HOMO: -7.02326 LUMO: 1.41227 factor:1 | 1 (-2.10197) | -1 | -1 |
| G: -5683.64846 HOMO: -6.59604 LUMO: 2.33746 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.28359 HOMO: -6.72121 LUMO: 1.43132 factor:1 | 1 (-1.26944) | -1 | -1 |
| G: -5683.64846 HOMO: -6.59604 LUMO: 2.33746 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.19991 HOMO: -6.51168 LUMO: 1.72520 factor:1 | 1 (-2.18575) | -1 | -1 |
| G: -5683.64846 HOMO: -6.59604 LUMO: 2.33746 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.93945 HOMO: -6.98516 LUMO: 1.92929 factor:1 | 1 (-0.92530) | 1 | 1 |
| G: -5683.64846 HOMO: -6.59604 LUMO: 2.33746 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.91873 HOMO: -6.92802 LUMO: 2.07895 factor:1 | 1 (-1.90458) | 1 | 1 |
| G: -5683.64846 HOMO: -6.59604 LUMO: 2.33746 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.19986 HOMO: -7.02326 LUMO: 1.86398 factor:1 | 1 (-1.18571) | 1 | 1 |
| G: -5683.64846 HOMO: -6.59604 LUMO: 2.33746 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.01496 HOMO: -6.82462 LUMO: 1.86670 factor:1 | 1 (-1.00081) | 1 | 1 |
| G: -5683.64846 HOMO: -6.59604 LUMO: 2.33746 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.50429 HOMO: -6.83278 LUMO: 1.71160 factor:1 | 1 (-2.49014) | 1 | 1 |
| G: -5683.64846 HOMO: -6.59604 LUMO: 2.33746 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.92357 HOMO: -6.62869 LUMO: 1.69527 factor:1 | 1 (-2.90941) | 1 | 1 |
| G: -5683.64846 HOMO: -6.59604 LUMO: 2.33746 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.36402 HOMO: -6.84094 LUMO: 1.27349 factor:1 | 1 (-2.34987) | -1 | -1 |
| G: -5683.64846 HOMO: -6.59604 LUMO: 2.33746 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.11069 HOMO: -7.07768 LUMO: 1.27621 factor:1 | 1 (-1.09654) | -1 | -1 |
| G: -5683.64846 HOMO: -6.59604 LUMO: 2.33746 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.95613 HOMO: -7.06135 LUMO: 1.55105 factor:1 | 1 (-0.94198) | -1 | -1 |
| G: -5683.64846 HOMO: -6.59604 LUMO: 2.33746 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.98492 HOMO: -6.94162 LUMO: 1.64629 factor:1 | 1 (-0.97077) | 1 | 1 |
| G: -5683.64846 HOMO: -6.59604 LUMO: 2.33746 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.08647 HOMO: -7.07224 LUMO: 1.65445 factor:1 | 1 (-1.07232) | 1 | 1 |
| G: -5683.64846 HOMO: -6.59604 LUMO: 2.33746 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.19442 HOMO: -6.68584 LUMO: 1.91296 factor:1 | 1 (-1.18027) | 1 | 1 |
| G: -5683.64846 HOMO: -6.59604 LUMO: 2.33746 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.31243 HOMO: -7.09129 LUMO: 1.73609 factor:1 | 1 (-1.29828) | 1 | 1 |
| G: -5683.64846 HOMO: -6.59604 LUMO: 2.33746 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.05071 HOMO: -7.01237 LUMO: 2.01092 factor:1 | 1 (-2.03655) | 1 | 1 |
| G: -5683.64846 HOMO: -6.59604 LUMO: 2.33746 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.09719 HOMO: -6.93618 LUMO: 1.63540 factor:1 | 1 (-1.08304) | 1 | 1 |
| G: -5683.64846 HOMO: -6.59604 LUMO: 2.33746 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.53806 HOMO: -6.98516 LUMO: 1.64629 factor:1 | 1 (-2.52391) | 1 | 1 |
| G: -5683.64846 HOMO: -6.59604 LUMO: 2.33746 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.89642 HOMO: -6.80285 LUMO: 1.95106 factor:1 | 1 (-1.88227) | 1 | 1 |
| G: -5683.64846 HOMO: -6.59604 LUMO: 2.33746 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.12118 HOMO: -6.76747 LUMO: 1.88303 factor:1 | 1 (-2.10703) | 1 | 1 |
| G: -5683.64846 HOMO: -6.59604 LUMO: 2.33746 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.58702 HOMO: -6.64230 LUMO: 1.90480 factor:1 | 1 (-2.57286) | 1 | 1 |
| G: -5683.64846 HOMO: -6.59604 LUMO: 2.33746 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.20524 HOMO: -6.93618 LUMO: 2.19324 factor:1 | 1 (-2.19109) | 1 | 1 |
| G: -5683.64846 HOMO: -6.59604 LUMO: 2.33746 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.72411 HOMO: -6.95523 LUMO: 1.80684 factor:1 | 1 (-2.70995) | 1 | 1 |
| G: -5683.64846 HOMO: -6.59604 LUMO: 2.33746 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.86842 HOMO: -6.66135 LUMO: 1.72792 factor:1 | 1 (-1.85427) | 1 | 1 |
| G: -5683.64846 HOMO: -6.59604 LUMO: 2.33746 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.96488 HOMO: -6.36202 LUMO: 1.89391 factor:1 | 1 (-1.95073) | -1 | -1 |
| G: -5683.64846 HOMO: -6.59604 LUMO: 2.33746 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.10546 HOMO: -7.03959 LUMO: 2.06262 factor:1 | 1 (-2.09130) | 1 | 1 |
| G: -5683.64846 HOMO: -6.59604 LUMO: 2.33746 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.54270 HOMO: -7.08584 LUMO: 2.01092 factor:1 | 1 (-1.52855) | 1 | 1 |
| G: -5683.64846 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.72539 HOMO: -7.06135 LUMO: 0.75376 factor:1 | 1 (-1.71124) | 1 | -1 |
| G: -5683.64846 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.60278 HOMO: -5.10213 LUMO: 0.77825 factor:1 | 1 (-1.58863) | -1 | -1 |
| G: -5683.64846 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.68093 HOMO: -5.84228 LUMO: 0.50341 factor:1 | 1 (-1.66678) | -1 | -1 |
| G: -5683.64846 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.03235 HOMO: -5.39874 LUMO: 0.68028 factor:1 | 1 (-1.01820) | -1 | -1 |
| G: -5683.64846 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.10936 HOMO: -5.16744 LUMO: 1.14832 factor:1 | 1 (-1.09520) | -1 | -1 |
| G: -5683.64846 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.05052 HOMO: -5.80963 LUMO: 0.35647 factor:1 | 1 (-1.03637) | -1 | -1 |
| G: -5683.64846 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.98486 HOMO: -5.02322 LUMO: 1.07213 factor:1 | 1 (-0.97071) | -1 | -1 |
| G: -5683.64846 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.00152 HOMO: -5.80963 LUMO: 0.56328 factor:1 | 1 (-0.98737) | -1 | -1 |
| G: -5683.64846 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.66905 HOMO: -5.45316 LUMO: 0.78369 factor:1 | 1 (-0.65490) | -1 | -1 |
| G: -5683.64846 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.36095 HOMO: -5.25452 LUMO: 0.82178 factor:1 | 1 (-1.34680) | -1 | -1 |
| G: -5683.64846 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.67718 HOMO: -5.21370 LUMO: 1.03947 factor:1 | 1 (-1.66302) | -1 | -1 |
| G: -5683.64846 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.73582 HOMO: -6.04365 LUMO: 0.31837 factor:1 | 1 (-0.72167) | -1 | -1 |
| G: -5683.64846 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.18583 HOMO: -5.86405 LUMO: 0.55511 factor:1 | 1 (-0.17168) | -1 | -1 |
| G: -5683.64846 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.21609 HOMO: -5.64908 LUMO: 0.71022 factor:1 | 1 (-0.20194) | -1 | -1 |
| G: -5683.64846 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.94764 HOMO: -5.94297 LUMO: 0.68301 factor:1 | 1 (-0.93349) | -1 | -1 |
| G: -5683.64846 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.15462 HOMO: -6.01916 LUMO: 0.56328 factor:1 | 1 (-0.14047) | -1 | -1 |
| G: -5683.64846 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.84473 HOMO: -6.05181 LUMO: 0.35103 factor:1 | -1 (0.16942) | -1 | -1 |
| G: -5683.64846 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.93727 HOMO: -6.08447 LUMO: 0.48436 factor:1 | 1 (-0.92312) | -1 | -1 |
| G: -5683.64846 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.90020 HOMO: -5.86950 LUMO: 0.36735 factor:1 | 1 (-1.88605) | -1 | -1 |
| G: -5683.64846 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.91254 HOMO: -5.33615 LUMO: 0.65852 factor:1 | 1 (-0.89838) | -1 | -1 |
| G: -5683.64846 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.13171 HOMO: -5.36064 LUMO: 0.86804 factor:1 | 1 (-2.11756) | -1 | -1 |
| G: -5683.64846 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.82854 HOMO: -5.74160 LUMO: 0.64491 factor:1 | 1 (-2.81439) | -1 | -1 |
| G: -5683.64846 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.98202 HOMO: -5.23003 LUMO: 0.66124 factor:1 | 1 (-2.96786) | -1 | -1 |
| G: -5683.64846 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.10728 HOMO: -5.77698 LUMO: 0.84083 factor:1 | 1 (-2.09313) | -1 | -1 |
| G: -5683.64846 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.98588 HOMO: -5.60555 LUMO: 0.84355 factor:1 | -1 (0.02827) | -1 | -1 |
| G: -5683.64846 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.86264 HOMO: -7.11578 LUMO: -1.62452 factor:1 | -1 (0.15151) | -1 | -1 |
| G: -5683.64846 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.02879 HOMO: -7.23279 LUMO: -1.63813 factor:1 | 1 (-0.01464) | -1 | -1 |
| G: -5683.64846 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.64396 HOMO: -6.68312 LUMO: -0.88709 factor:1 | 1 (-0.62981) | -1 | -1 |
| G: -5683.64846 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.68145 HOMO: -6.99333 LUMO: -0.88709 factor:1 | 1 (-1.66730) | -1 | -1 |
| G: -5683.64846 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.54645 HOMO: -7.40694 LUMO: 0.11973 factor:1 | 1 (-1.53230) | 1 | 1 |
| G: -5683.64846 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.63307 HOMO: -6.74026 LUMO: -0.72927 factor:1 | 1 (-0.61892) | -1 | -1 |
| G: -5683.64846 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.67223 HOMO: -6.67223 LUMO: -0.70750 factor:1 | 1 (-0.65808) | -1 | -1 |
| G: -5683.64846 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.65280 HOMO: -7.06952 LUMO: -1.40139 factor:1 | 1 (-0.63865) | -1 | -1 |
| G: -5683.64846 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.75874 HOMO: -7.21374 LUMO: -1.13199 factor:1 | 1 (-0.74459) | -1 | -1 |
| G: -5683.64846 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.47457 HOMO: -6.54706 LUMO: -1.34424 factor:1 | 1 (-0.46042) | -1 | -1 |
| G: -5683.64846 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.33994 HOMO: -7.51851 LUMO: -1.05852 factor:1 | 1 (-1.32579) | -1 | -1 |
| G: -5683.64846 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.10616 HOMO: -7.07224 LUMO: -1.89391 factor:1 | 1 (-2.09201) | -1 | -1 |
| G: -5683.64846 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.17234 HOMO: -6.65863 LUMO: -0.46804 factor:1 | 1 (-2.15819) | -1 | -1 |
| G: -5683.64846 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.23996 HOMO: -7.24367 LUMO: 0.29388 factor:1 | 1 (-2.22581) | 1 | 1 |
| G: -5683.64846 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.27207 HOMO: -7.02326 LUMO: -0.87893 factor:1 | 1 (-2.25792) | -1 | -1 |
| G: -5683.64846 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.32775 HOMO: -6.88176 LUMO: 0.71566 factor:1 | 1 (-2.31359) | -1 | -1 |
| G: -5683.64846 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.88825 HOMO: -6.46543 LUMO: 1.01498 factor:1 | 1 (-2.87409) | -1 | -1 |
| G: -5683.64846 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.98220 HOMO: -6.30760 LUMO: 0.17687 factor:1 | 1 (-0.96805) | -1 | -1 |
| G: -5683.64846 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.04886 HOMO: -6.73210 LUMO: -1.06941 factor:1 | 1 (-1.03471) | -1 | -1 |
| G: -5683.64846 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.72612 HOMO: -6.83550 LUMO: -0.75920 factor:1 | 1 (-2.71197) | -1 | -1 |
| G: -5683.64846 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.02189 HOMO: -6.94707 LUMO: 0.42178 factor:1 | 1 (-2.00774) | -1 | -1 |
| G: -5683.64846 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.62680 HOMO: -6.77019 LUMO: -0.38096 factor:1 | 1 (-2.61265) | -1 | -1 |
| G: -5683.64846 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.94118 HOMO: -7.34163 LUMO: 0.35103 factor:1 | 1 (-1.92703) | 1 | 1 |
| G: -5683.64846 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.60816 HOMO: -6.87632 LUMO: -0.87349 factor:1 | 1 (-2.59401) | -1 | -1 |
| G: -5683.64846 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.52232 HOMO: -7.06952 LUMO: -1.47214 factor:1 | 1 (-1.50816) | -1 | -1 |
| G: -5683.64846 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.51532 HOMO: -6.58788 LUMO: -0.37824 factor:1 | 1 (-1.50117) | -1 | -1 |
| G: -5683.64846 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.53657 HOMO: -6.92802 LUMO: -1.24900 factor:1 | 1 (-1.52242) | -1 | -1 |
| G: -5683.64846 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.10706 HOMO: -7.01237 LUMO: -1.31975 factor:1 | 1 (-2.09291) | -1 | -1 |
| G: -5683.64846 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.14936 HOMO: -6.74842 LUMO: 0.45987 factor:1 | 1 (-1.13520) | -1 | -1 |
| G: -5683.64846 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.95849 HOMO: -6.53890 LUMO: 0.94424 factor:1 | 1 (-1.94434) | -1 | -1 |
| G: -5683.64846 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.20272 HOMO: -6.52257 LUMO: -0.66940 factor:1 | 1 (-1.18857) | -1 | -1 |
| G: -5683.64846 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.93446 HOMO: -6.56883 LUMO: -1.48302 factor:1 | 1 (-1.92031) | -1 | -1 |
| G: -5683.64846 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.27635 HOMO: -7.21646 LUMO: 0.13061 factor:1 | 1 (-1.26220) | 1 | 1 |
| G: -5683.64846 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.90423 HOMO: -6.62597 LUMO: -0.64763 factor:1 | 1 (-1.89008) | -1 | -1 |
| G: -5683.64846 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.08797 HOMO: -7.38789 LUMO: 0.31021 factor:1 | 1 (-1.07382) | 1 | 1 |
| G: -5683.64846 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.66918 HOMO: -6.74570 LUMO: -0.70750 factor:1 | 1 (-1.65502) | -1 | -1 |
| G: -5683.64846 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.87506 HOMO: -6.95251 LUMO: -1.25989 factor:1 | 1 (-1.86091) | -1 | -1 |
| G: -5683.64846 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.54311 HOMO: -7.13483 LUMO: -0.76736 factor:1 | 1 (-0.52896) | -1 | -1 |
| G: -5683.64846 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.08397 HOMO: -6.93618 LUMO: -1.24628 factor:1 | 1 (-1.06982) | -1 | -1 |
| G: -5683.64846 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.60521 HOMO: -7.03686 LUMO: 0.26395 factor:1 | 1 (-0.59106) | -1 | -1 |
| G: -5683.64846 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.47226 HOMO: -6.52257 LUMO: -0.84355 factor:1 | 1 (-0.45810) | -1 | -1 |
| G: -5683.64846 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.91967 HOMO: -6.83278 LUMO: -0.49525 factor:1 | 1 (-0.90551) | -1 | -1 |
| G: -5683.64846 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.30173 HOMO: -7.18381 LUMO: -1.64629 factor:1 | 1 (-2.28758) | -1 | -1 |
| G: -5683.64846 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.39954 HOMO: -6.74842 LUMO: -0.81090 factor:1 | 1 (-1.38539) | -1 | -1 |
| G: -5683.64846 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.98184 HOMO: -7.09401 LUMO: -0.92519 factor:1 | 1 (-0.96769) | -1 | -1 |
| G: -5683.64846 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.81077 HOMO: -7.20285 LUMO: -0.81634 factor:1 | -1 (0.20338) | -1 | -1 |
| G: -5683.64846 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.89584 HOMO: -6.72665 LUMO: 0.77008 factor:1 | -1 (0.11832) | -1 | -1 |
| G: -5683.64846 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.57365 HOMO: -6.80829 LUMO: 0.86532 factor:1 | -1 (0.44050) | -1 | -1 |
| G: -5683.64846 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.94457 HOMO: -6.20964 LUMO: 0.99866 factor:1 | -1 (0.06958) | -1 | -1 |
| G: -5683.64846 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.54587 HOMO: -6.52801 LUMO: 1.07757 factor:1 | -1 (0.46828) | -1 | -1 |
| G: -5683.64846 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.79397 HOMO: -6.74298 LUMO: -0.67756 factor:1 | 1 (-1.77982) | -1 | -1 |
| G: -5683.64846 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.93036 HOMO: -7.43959 LUMO: 0.03265 factor:1 | 1 (-0.91621) | 1 | 1 |
| G: -5683.64846 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.02108 HOMO: -6.46815 LUMO: -0.29933 factor:1 | 1 (-1.00693) | -1 | -1 |
| G: -5683.64846 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.63343 HOMO: -6.70489 LUMO: -0.97145 factor:1 | 1 (-0.61928) | -1 | -1 |
| G: -5683.64846 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.16242 HOMO: -6.30216 LUMO: -1.39322 factor:1 | 1 (-1.14827) | -1 | -1 |
| G: -5683.64846 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.29418 HOMO: -7.01782 LUMO: -1.07485 factor:1 | 1 (-1.28002) | -1 | -1 |
| G: -5683.64846 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.50801 HOMO: -6.93074 LUMO: 0.25851 factor:1 | 1 (-0.49386) | -1 | -1 |
| G: -5683.64846 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.59250 HOMO: -7.07224 LUMO: 0.09524 factor:1 | 1 (-0.57835) | 1 | 1 |
| G: -5683.64846 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.90331 HOMO: -6.62325 LUMO: -0.45443 factor:1 | 1 (-0.88916) | -1 | -1 |
| G: -5683.64846 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.19026 HOMO: -7.09945 LUMO: -1.20274 factor:1 | 1 (-1.17610) | -1 | -1 |
| G: -5683.64846 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.61737 HOMO: -6.56067 LUMO: -1.39322 factor:1 | 1 (-0.60322) | -1 | -1 |
| G: -5683.64846 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.99578 HOMO: -6.75387 LUMO: -0.72654 factor:1 | -1 (0.01837) | -1 | -1 |
| G: -5683.64846 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.05127 HOMO: -6.28583 LUMO: -2.35651 factor:1 | 1 (-0.03712) | -1 | -1 |
| G: -5683.64846 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11946.00938 HOMO: -6.55522 LUMO: -1.33608 factor:1 | -1 (2.00477) | -1 | -1 |
| G: -5683.64846 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11946.03033 HOMO: -7.19741 LUMO: -0.93607 factor:1 | -1 (1.98382) | -1 | -1 |
| G: -5683.64846 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11946.31091 HOMO: -6.39740 LUMO: -1.14832 factor:1 | -1 (1.70324) | -1 | -1 |
| G: -5683.64846 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11945.65326 HOMO: -7.11850 LUMO: -0.97417 factor:1 | -1 (2.36089) | -1 | -1 |
| G: -5683.64846 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11945.99025 HOMO: -6.57699 LUMO: -1.14016 factor:1 | -1 (2.02390) | -1 | -1 |
| G: -5683.64846 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.01498 HOMO: -6.57699 LUMO: -1.31975 factor:1 | -1 (0.99917) | -1 | -1 |
| G: -5683.64846 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.07299 HOMO: -6.69128 LUMO: -0.76736 factor:1 | -1 (0.94116) | -1 | -1 |
| G: -5683.64846 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11946.71513 HOMO: -7.25728 LUMO: 0.29660 factor:1 | -1 (1.29902) | 1 | 1 |
| G: -5683.64846 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11946.86564 HOMO: -6.37019 LUMO: -0.95240 factor:1 | -1 (1.14851) | -1 | -1 |
| G: -5683.64846 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11946.87138 HOMO: -6.48447 LUMO: -0.55511 factor:1 | -1 (1.14277) | -1 | -1 |
| G: -5683.64846 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.97526 HOMO: -6.37291 LUMO: -0.78641 factor:1 | 1 (-0.96111) | -1 | -1 |
| G: -5683.64846 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.43710 HOMO: -6.65863 LUMO: -0.69933 factor:1 | 1 (-0.42295) | -1 | -1 |
| G: -5683.64846 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.02674 HOMO: -6.44638 LUMO: -0.16055 factor:1 | 1 (-1.01259) | -1 | -1 |
| G: -5683.64846 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.00960 HOMO: -6.41917 LUMO: -0.20136 factor:1 | 1 (-0.99545) | -1 | -1 |
| G: -5683.64846 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.44287 HOMO: -7.33347 LUMO: 0.12789 factor:1 | 1 (-0.42872) | 1 | 1 |
| G: -5683.64846 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.16699 HOMO: -6.70489 LUMO: -0.52518 factor:1 | 1 (-1.15284) | -1 | -1 |
| G: -5683.64846 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.36034 HOMO: -7.25183 LUMO: 0.32109 factor:1 | 1 (-0.34618) | 1 | 1 |
| G: -5683.64846 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.93899 HOMO: -7.29265 LUMO: 0.28028 factor:1 | 1 (-0.92483) | 1 | 1 |
| G: -5683.64846 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.04626 HOMO: -6.57155 LUMO: -0.51702 factor:1 | 1 (-0.03211) | -1 | -1 |
| G: -5683.64846 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.44404 HOMO: -7.08040 LUMO: 0.39729 factor:1 | 1 (-0.42989) | 1 | 1 |
| G: -5683.64846 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.41729 HOMO: -6.24501 LUMO: -0.44627 factor:1 | 1 (-0.40314) | -1 | -1 |
| G: -5683.64846 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.10500 HOMO: -6.73754 LUMO: -0.45443 factor:1 | 1 (-1.09085) | -1 | -1 |
| G: -5683.64846 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.05108 HOMO: -6.24501 LUMO: 0.38096 factor:1 | 1 (-0.03693) | -1 | -1 |
| G: -5683.64846 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.02633 HOMO: -6.86815 LUMO: -0.91974 factor:1 | 1 (-1.01218) | -1 | -1 |
| G: -5683.64846 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.81278 HOMO: -7.40150 LUMO: 0.36191 factor:1 | 1 (-0.79863) | 1 | 1 |
| G: -5683.64846 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.58554 HOMO: -6.44094 LUMO: -0.64219 factor:1 | 1 (-0.57138) | -1 | -1 |
| G: -5683.64846 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11946.72455 HOMO: -6.69944 LUMO: -0.80001 factor:1 | -1 (1.28960) | -1 | -1 |
| G: -5683.64846 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11946.65873 HOMO: -6.61509 LUMO: -0.70750 factor:1 | -1 (1.35543) | -1 | -1 |
| G: -5683.64846 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11946.75263 HOMO: -7.52123 LUMO: 0.06803 factor:1 | -1 (1.26152) | 1 | 1 |
| G: -5683.64846 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.10878 HOMO: -7.34163 LUMO: 0.30477 factor:1 | 1 (-1.09463) | 1 | 1 |
| G: -5683.64846 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.84600 HOMO: -6.68584 LUMO: -0.78641 factor:1 | 1 (-0.83185) | -1 | -1 |
| G: -5683.64846 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.16396 HOMO: -6.53890 LUMO: -0.50885 factor:1 | 1 (-2.14981) | -1 | -1 |
| G: -5683.64846 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.27752 HOMO: -6.75659 LUMO: -0.68845 factor:1 | 1 (-1.26337) | -1 | -1 |
| G: -5683.64846 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.08698 HOMO: -7.08857 LUMO: 0.43266 factor:1 | 1 (-2.07283) | 1 | 1 |
| G: -5683.64846 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.67220 HOMO: -6.28583 LUMO: -0.46804 factor:1 | 1 (-1.65804) | -1 | -1 |
| G: -5683.64846 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.95626 HOMO: -6.50080 LUMO: -0.24762 factor:1 | 1 (-1.94210) | -1 | -1 |
| G: -5683.64846 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.19894 HOMO: -6.45454 LUMO: -0.58504 factor:1 | 1 (-1.18478) | -1 | -1 |
| G: -5683.64846 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.35605 HOMO: -7.20558 LUMO: 0.20953 factor:1 | 1 (-1.34190) | 1 | 1 |
| G: -5683.64846 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.87722 HOMO: -6.35930 LUMO: -0.20681 factor:1 | 1 (-0.86306) | -1 | -1 |
| G: -5683.64846 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.09270 HOMO: -6.36202 LUMO: -0.14422 factor:1 | 1 (-1.07855) | -1 | -1 |
| G: -5683.64846 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.75685 HOMO: -6.20692 LUMO: 1.97827 factor:1 | 1 (-1.74270) | -1 | -1 |
| G: -5683.64846 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.75622 HOMO: -6.48719 LUMO: 1.74153 factor:1 | 1 (-1.74207) | -1 | -1 |
| G: -5683.64846 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.02084 HOMO: -6.84638 LUMO: 1.88575 factor:1 | 1 (-1.00669) | -1 | -1 |
| G: -5683.64846 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.19523 HOMO: -5.90759 LUMO: 2.00820 factor:1 | 1 (-1.18108) | -1 | -1 |
| G: -5683.64846 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11946.82175 HOMO: -6.56339 LUMO: 1.99732 factor:1 | -1 (1.19240) | -1 | -1 |
| G: -5683.64846 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.91181 HOMO: -6.20692 LUMO: 1.75241 factor:1 | -1 (0.10234) | -1 | -1 |
| G: -5683.64846 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.05004 HOMO: -6.16882 LUMO: 1.94017 factor:1 | 1 (-0.03589) | -1 | -1 |
| G: -5683.64846 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.55727 HOMO: -6.80829 LUMO: 1.78507 factor:1 | -1 (0.45688) | -1 | -1 |
| G: -5683.64846 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.59484 HOMO: -6.58243 LUMO: 1.78235 factor:1 | 1 (-0.58069) | -1 | -1 |
| G: -5683.64846 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.55286 HOMO: -5.85045 LUMO: 1.82316 factor:1 | -1 (0.46129) | -1 | -1 |
| G: -5683.64846 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.82655 HOMO: -5.93752 LUMO: 1.56465 factor:1 | 1 (-0.81240) | -1 | -1 |
| G: -5683.64846 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.75642 HOMO: -6.59604 LUMO: -0.53334 factor:1 | 1 (-0.74227) | -1 | -1 |
| G: -5683.64846 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.70690 HOMO: -7.06135 LUMO: 0.29660 factor:1 | 1 (-0.69275) | 1 | 1 |
| G: -5683.64846 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.11412 HOMO: -6.50352 LUMO: 1.61908 factor:1 | 1 (-1.09997) | -1 | -1 |
| G: -5683.64846 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.84023 HOMO: -6.68040 LUMO: -0.60681 factor:1 | 1 (-1.82607) | -1 | -1 |
| G: -5683.64846 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.97324 HOMO: -6.93618 LUMO: -1.09662 factor:1 | 1 (-0.95909) | -1 | -1 |
| G: -5683.64846 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.90020 HOMO: -6.72121 LUMO: -1.14016 factor:1 | 1 (-1.88605) | -1 | -1 |
| G: -5683.64846 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.16693 HOMO: -7.12394 LUMO: -1.24900 factor:1 | 1 (-1.15278) | -1 | -1 |
| G: -5683.64846 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.91177 HOMO: -6.71305 LUMO: -0.71566 factor:1 | 1 (-0.89762) | -1 | -1 |
| G: -5683.64846 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.31646 HOMO: -7.09401 LUMO: -0.86532 factor:1 | 1 (-1.30231) | -1 | -1 |
| G: -5683.64846 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.46246 HOMO: -7.08584 LUMO: -0.92519 factor:1 | 1 (-0.44831) | -1 | -1 |
| G: -5683.64846 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.88578 HOMO: -7.05591 LUMO: 0.11973 factor:1 | 1 (-1.87163) | -1 | -1 |
| G: -5683.64846 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.15771 HOMO: -7.14843 LUMO: -1.58370 factor:1 | 1 (-1.14356) | -1 | -1 |
| G: -5683.64846 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.93411 HOMO: -7.36884 LUMO: -1.97010 factor:1 | 1 (-0.91996) | -1 | -1 |
| G: -5683.64846 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.84062 HOMO: -6.81373 LUMO: -1.72248 factor:1 | 1 (-0.82646) | -1 | -1 |
| G: -5683.64846 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.34560 HOMO: -6.87360 LUMO: -1.03947 factor:1 | 1 (-2.33144) | -1 | -1 |
| G: -5683.64846 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.62049 HOMO: -7.02870 LUMO: -0.87349 factor:1 | 1 (-1.60634) | -1 | -1 |
| G: -5683.64846 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.15023 HOMO: -7.16476 LUMO: -1.18097 factor:1 | 1 (-1.13608) | -1 | -1 |
| G: -5683.64846 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.00990 HOMO: -7.51851 LUMO: 0.07891 factor:1 | 1 (-0.99575) | 1 | 1 |
| G: -5683.64846 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.29154 HOMO: -7.04231 LUMO: -0.83539 factor:1 | 1 (-0.27739) | -1 | -1 |
| G: -5683.64846 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.93635 HOMO: -6.83278 LUMO: -0.60137 factor:1 | -1 (0.07780) | -1 | -1 |
| G: -5683.64846 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.18806 HOMO: -6.89809 LUMO: -1.19186 factor:1 | 1 (-0.17391) | -1 | -1 |
| G: -5683.64846 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.35944 HOMO: -7.16476 LUMO: -0.79185 factor:1 | 1 (-0.34529) | -1 | -1 |
| G: -5683.64846 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.75951 HOMO: -6.97156 LUMO: -1.25444 factor:1 | -1 (0.25464) | -1 | -1 |
| G: -5683.64846 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.38970 HOMO: -6.84366 LUMO: -0.88437 factor:1 | 1 (-0.37554) | -1 | -1 |
| G: -5683.64846 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.56211 HOMO: -6.91986 LUMO: -1.12655 factor:1 | 1 (-0.54796) | -1 | -1 |
| G: -5683.64846 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.54599 HOMO: -6.49536 LUMO: -0.29660 factor:1 | 1 (-1.53184) | -1 | -1 |
| G: -5683.64846 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.24244 HOMO: -6.74842 LUMO: 0.42450 factor:1 | 1 (-2.22829) | -1 | -1 |
| G: -5683.64846 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.83378 HOMO: -7.34435 LUMO: 0.32109 factor:1 | 1 (-1.81963) | 1 | 1 |
| G: -5683.64846 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.40672 HOMO: -7.16476 LUMO: 0.28572 factor:1 | 1 (-1.39257) | 1 | 1 |
| G: -5683.64846 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.02900 HOMO: -6.74298 LUMO: -0.43538 factor:1 | 1 (-1.01485) | -1 | -1 |
| G: -5683.64846 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.77281 HOMO: -7.19469 LUMO: -1.61091 factor:1 | 1 (-0.75865) | -1 | -1 |
| G: -5683.64846 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.85887 HOMO: -7.35252 LUMO: -1.78235 factor:1 | 1 (-0.84472) | -1 | -1 |
| G: -5683.64846 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.79498 HOMO: -7.25456 LUMO: -1.66806 factor:1 | 1 (-0.78083) | -1 | -1 |
| G: -5683.64846 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.69394 HOMO: -7.54844 LUMO: -1.07213 factor:1 | 1 (-1.67979) | -1 | -1 |
| G: -5683.64846 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.46523 HOMO: -7.21918 LUMO: -1.55377 factor:1 | 1 (-0.45108) | -1 | -1 |
| G: -5683.64846 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.76908 HOMO: -7.01782 LUMO: -1.60547 factor:1 | 1 (-0.75493) | -1 | -1 |
| G: -5683.64846 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.31277 HOMO: -7.21646 LUMO: -1.53472 factor:1 | 1 (-0.29862) | -1 | -1 |
| G: -5683.64846 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.92435 HOMO: -6.73754 LUMO: -1.37417 factor:1 | -1 (0.08980) | -1 | -1 |
| G: -5683.64846 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.05878 HOMO: -6.78924 LUMO: 0.66396 factor:1 | 1 (-0.04463) | -1 | -1 |
| G: -5683.64846 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.57531 HOMO: -6.82734 LUMO: 0.61226 factor:1 | -1 (0.43884) | -1 | -1 |
| G: -5683.64846 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.90220 HOMO: -6.74026 LUMO: 0.65579 factor:1 | -1 (0.11195) | -1 | -1 |
| G: -5683.64846 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.96280 HOMO: -7.10489 LUMO: -1.30887 factor:1 | 1 (-0.94864) | -1 | -1 |
| G: -5683.64846 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.15719 HOMO: -7.05047 LUMO: 0.42722 factor:1 | 1 (-1.14304) | -1 | -1 |
| G: -5683.64846 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.00250 HOMO: -6.61237 LUMO: 1.30887 factor:1 | 1 (-0.98834) | -1 | -1 |
| G: -5683.64846 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.48896 HOMO: -7.05863 LUMO: 0.59049 factor:1 | 1 (-0.47481) | -1 | -1 |
| G: -5683.64846 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.16163 HOMO: -6.26406 LUMO: 0.78641 factor:1 | 1 (-1.14748) | -1 | -1 |
| G: -5683.64846 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.76059 HOMO: -6.70489 LUMO: 0.67756 factor:1 | 1 (-0.74644) | -1 | -1 |
| G: -5683.64846 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.43514 HOMO: -6.78652 LUMO: -0.94968 factor:1 | 1 (-0.42099) | -1 | -1 |
| G: -5683.64846 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.05814 HOMO: -6.36202 LUMO: -0.94424 factor:1 | 1 (-1.04399) | -1 | -1 |
| G: -5683.64846 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.79856 HOMO: -6.81645 LUMO: -1.09934 factor:1 | -1 (0.21560) | -1 | -1 |
| G: -5683.64846 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.83151 HOMO: -7.07224 LUMO: 0.85988 factor:1 | -1 (0.18264) | 1 | 1 |
| G: -5683.64846 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.15595 HOMO: -7.02326 LUMO: 1.10206 factor:1 | 1 (-0.14180) | -1 | -1 |
| G: -5683.64846 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.87529 HOMO: -6.71305 LUMO: 0.84627 factor:1 | -1 (0.13886) | -1 | -1 |
| G: -5683.64846 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.52467 HOMO: -7.27360 LUMO: 0.88165 factor:1 | -1 (0.48948) | 1 | 1 |
| G: -5683.64846 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.15930 HOMO: -6.84911 LUMO: 0.59865 factor:1 | 1 (-0.14515) | -1 | -1 |
| G: -5683.64846 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.85355 HOMO: -6.75114 LUMO: -2.49801 factor:1 | -1 (0.16060) | -1 | -1 |
| G: -5683.64846 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.62767 HOMO: -6.97156 LUMO: 0.53606 factor:1 | -1 (0.38648) | -1 | -1 |
| G: -5683.64846 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.80206 HOMO: -6.54434 LUMO: 0.73199 factor:1 | 1 (-0.78791) | -1 | -1 |
| G: -5683.64846 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.74807 HOMO: -6.21236 LUMO: 0.99866 factor:1 | 1 (-0.73392) | -1 | -1 |
| G: -5683.64846 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.74802 HOMO: -6.34025 LUMO: 0.50341 factor:1 | 1 (-0.73386) | -1 | -1 |
| G: -5683.64846 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.95673 HOMO: -6.59876 LUMO: -0.69389 factor:1 | 1 (-0.94258) | -1 | -1 |
| G: -5683.64846 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.10447 HOMO: -6.54978 LUMO: -1.00682 factor:1 | 1 (-0.09031) | -1 | -1 |
| G: -5683.64846 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.06133 HOMO: -6.82462 LUMO: -0.98777 factor:1 | 1 (-1.04718) | -1 | -1 |
| G: -5683.64846 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.35051 HOMO: -6.85455 LUMO: -0.68573 factor:1 | 1 (-0.33636) | -1 | -1 |
| G: -5683.64846 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.15620 HOMO: -7.55388 LUMO: -0.03265 factor:1 | 1 (-0.14204) | 1 | 1 |
| G: -5683.64846 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.65049 HOMO: -6.77019 LUMO: -0.71838 factor:1 | 1 (-0.63634) | -1 | -1 |
| G: -5683.64846 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.71284 HOMO: -6.84911 LUMO: -1.25444 factor:1 | -1 (0.30131) | -1 | -1 |
| G: -5683.64846 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.99746 HOMO: -6.95251 LUMO: -1.03675 factor:1 | 1 (-0.98331) | -1 | -1 |
| G: -5683.64846 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.33367 HOMO: -6.80829 LUMO: -0.77280 factor:1 | 1 (-0.31952) | -1 | -1 |
| G: -5683.64846 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.09549 HOMO: -6.94162 LUMO: -0.94151 factor:1 | 1 (-0.08133) | -1 | -1 |
| G: -5683.64846 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.09899 HOMO: -6.89809 LUMO: -0.90886 factor:1 | 1 (-1.08484) | -1 | -1 |
| G: -5683.64846 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.76731 HOMO: -6.85183 LUMO: -0.88981 factor:1 | 1 (-0.75316) | -1 | -1 |
| G: -5683.64846 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.78130 HOMO: -6.51985 LUMO: -0.84627 factor:1 | 1 (-0.76714) | -1 | -1 |
| G: -5683.64846 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.26994 HOMO: -6.83278 LUMO: -1.08029 factor:1 | 1 (-0.25579) | -1 | -1 |
| G: -5683.64846 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.35385 HOMO: -6.91986 LUMO: 0.66396 factor:1 | 1 (-1.33970) | -1 | -1 |
| G: -5683.64846 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.75152 HOMO: -6.94162 LUMO: 0.50885 factor:1 | 1 (-1.73737) | -1 | -1 |
| G: -5683.64846 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.44132 HOMO: -6.94435 LUMO: 0.80546 factor:1 | 1 (-0.42716) | -1 | -1 |
| G: -5683.64846 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.92837 HOMO: -6.74298 LUMO: -0.81634 factor:1 | 1 (-0.91422) | -1 | -1 |
| G: -5683.64846 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.54978 HOMO: -7.04503 LUMO: 1.15921 factor:1 | 1 (-0.53563) | -1 | -1 |
| G: -5683.64846 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.44855 HOMO: -6.76475 LUMO: 0.75920 factor:1 | 1 (-0.43440) | -1 | -1 |
| G: -5683.64846 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.33051 HOMO: -7.05047 LUMO: 0.68845 factor:1 | 1 (-0.31636) | -1 | -1 |
| G: -5683.64846 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.48804 HOMO: -7.12666 LUMO: 0.60681 factor:1 | 1 (-0.47389) | 1 | 1 |
| G: -5683.64846 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.41174 HOMO: -6.90897 LUMO: -1.22723 factor:1 | 1 (-0.39759) | -1 | -1 |
| G: -5683.64846 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.65069 HOMO: -7.10761 LUMO: 0.58232 factor:1 | -1 (0.36346) | 1 | 1 |
| G: -5683.64846 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.23845 HOMO: -6.57427 LUMO: 0.71294 factor:1 | 1 (-1.22429) | -1 | -1 |
| G: -5683.64846 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.65332 HOMO: -6.22597 LUMO: 0.99322 factor:1 | 1 (-0.63917) | -1 | -1 |
| G: -5683.64846 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.30563 HOMO: -6.83550 LUMO: -0.77825 factor:1 | 1 (-1.29148) | -1 | -1 |
| G: -5683.64846 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.14329 HOMO: -7.14843 LUMO: 0.44627 factor:1 | 1 (-1.12914) | 1 | 1 |
| G: -5683.64846 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.64252 HOMO: -7.08040 LUMO: 0.78913 factor:1 | 1 (-0.62837) | 1 | 1 |
| G: -5683.64846 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.12234 HOMO: -6.81373 LUMO: -0.93879 factor:1 | 1 (-1.10818) | -1 | -1 |
| G: -5683.64846 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.23189 HOMO: -6.95251 LUMO: 0.22585 factor:1 | 1 (-1.21774) | -1 | -1 |
| G: -5683.64846 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.60118 HOMO: -7.13483 LUMO: -1.25444 factor:1 | 1 (-0.58703) | -1 | -1 |
| G: -5683.64846 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.09127 HOMO: -6.37835 LUMO: -1.54289 factor:1 | 1 (-0.07712) | -1 | -1 |
| G: -5683.64846 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11946.76387 HOMO: -6.53617 LUMO: -1.43948 factor:1 | -1 (1.25028) | -1 | -1 |
| G: -5683.64846 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.25117 HOMO: -6.38379 LUMO: 0.16055 factor:1 | -1 (0.76298) | -1 | -1 |
| G: -5683.64846 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11946.55042 HOMO: -6.53617 LUMO: 0.15783 factor:1 | -1 (1.46373) | -1 | -1 |
| G: -5683.64846 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11946.53129 HOMO: -6.79740 LUMO: -0.17960 factor:1 | -1 (1.48286) | -1 | -1 |
| G: -5683.64846 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11946.83432 HOMO: -6.26678 LUMO: -0.41361 factor:1 | -1 (1.17983) | -1 | -1 |
| G: -5683.64846 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.12693 HOMO: -6.35658 LUMO: -0.24218 factor:1 | 1 (-1.11278) | -1 | -1 |
| G: -5683.64846 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.75980 HOMO: -6.48175 LUMO: -0.71566 factor:1 | 1 (-0.74565) | -1 | -1 |
| G: -5683.64846 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.19627 HOMO: -6.21508 LUMO: -0.40001 factor:1 | 1 (-1.18212) | -1 | -1 |
| G: -5683.64846 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.89041 HOMO: -6.51985 LUMO: -0.32654 factor:1 | 1 (-0.87626) | -1 | -1 |
| G: -5683.64846 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.07494 HOMO: -6.45182 LUMO: -0.66396 factor:1 | 1 (-0.06079) | -1 | -1 |
| G: -5683.64846 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.36918 HOMO: -6.51441 LUMO: -0.65307 factor:1 | 1 (-0.35503) | -1 | -1 |
| G: -5683.64846 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.90283 HOMO: -6.57971 LUMO: -0.92519 factor:1 | -1 (0.11132) | -1 | -1 |
| G: -5683.64846 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.69327 HOMO: -6.67223 LUMO: -0.58232 factor:1 | 1 (-0.67911) | -1 | -1 |
| G: -5683.64846 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.21348 HOMO: -6.10351 LUMO: -0.45987 factor:1 | 1 (-0.19932) | -1 | -1 |
| G: -5683.64846 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.19488 HOMO: -6.13889 LUMO: -0.50341 factor:1 | 1 (-1.18073) | -1 | -1 |
| G: -5683.64846 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.26158 HOMO: -6.63141 LUMO: -0.28300 factor:1 | 1 (-1.24742) | -1 | -1 |
| G: -5683.64846 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.80025 HOMO: -6.37563 LUMO: -0.22858 factor:1 | 1 (-1.78610) | -1 | -1 |
| G: -5683.64846 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.76605 HOMO: -6.37019 LUMO: 0.11429 factor:1 | 1 (-1.75190) | -1 | -1 |
| G: -5683.64846 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.59355 HOMO: -6.23957 LUMO: 0.28844 factor:1 | -1 (0.42061) | -1 | -1 |
| G: -5683.64846 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.22857 HOMO: -6.41372 LUMO: -0.53879 factor:1 | 1 (-1.21442) | -1 | -1 |
| G: -5683.64846 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.24795 HOMO: -7.06680 LUMO: 0.32654 factor:1 | 1 (-0.23380) | 1 | 1 |
| G: -5683.64846 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.02952 HOMO: -6.50896 LUMO: -0.73743 factor:1 | 1 (-1.01537) | -1 | -1 |
| G: -5683.64846 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.72589 HOMO: -6.42189 LUMO: -0.28572 factor:1 | 1 (-0.71174) | -1 | -1 |
| G: -5683.64846 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.28215 HOMO: -6.79740 LUMO: -0.25851 factor:1 | 1 (-1.26800) | -1 | -1 |
| G: -5683.64846 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.05610 HOMO: -6.32393 LUMO: 0.17960 factor:1 | 1 (-1.04195) | -1 | -1 |
| G: -5683.64846 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.01354 HOMO: -6.65046 LUMO: 0.03537 factor:1 | 1 (-0.99939) | -1 | -1 |
| G: -5683.64846 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.43367 HOMO: -6.60148 LUMO: 0.07619 factor:1 | 1 (-0.41952) | -1 | -1 |
| G: -5683.64846 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.16838 HOMO: -6.57971 LUMO: 0.11429 factor:1 | 1 (-1.15423) | -1 | -1 |
| G: -5683.64846 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.10201 HOMO: -6.88448 LUMO: -1.21907 factor:1 | 1 (-1.08786) | -1 | -1 |
| G: -5683.64846 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.10783 HOMO: -6.97700 LUMO: 0.36463 factor:1 | 1 (-1.09368) | -1 | -1 |
| G: -5683.64846 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.20170 HOMO: -6.73210 LUMO: -0.84083 factor:1 | -1 (0.81245) | -1 | -1 |
| G: -5683.64846 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.15700 HOMO: -6.21236 LUMO: -0.68845 factor:1 | 1 (-1.14285) | -1 | -1 |
| G: -5683.64846 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11946.87285 HOMO: -6.35658 LUMO: -0.82995 factor:1 | -1 (1.14130) | -1 | -1 |
| G: -5683.64846 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.00586 HOMO: -6.75114 LUMO: -0.94424 factor:1 | -1 (1.00829) | -1 | -1 |
| G: -5683.64846 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.06151 HOMO: -6.74026 LUMO: -1.46125 factor:1 | -1 (0.95264) | -1 | -1 |
| G: -5683.64846 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.35291 HOMO: -7.06952 LUMO: 0.91974 factor:1 | 1 (-0.33875) | 1 | 1 |
| G: -5683.64846 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.09217 HOMO: -7.08857 LUMO: 0.74559 factor:1 | 1 (-0.07802) | 1 | 1 |
| G: -5683.64846 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.08219 HOMO: -6.74298 LUMO: 1.03131 factor:1 | -1 (0.93196) | -1 | -1 |
| G: -5683.64846 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.12260 HOMO: -6.74842 LUMO: -1.77962 factor:1 | -1 (0.89155) | -1 | -1 |
| G: -5683.64846 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.72424 HOMO: -6.82462 LUMO: -1.61908 factor:1 | -1 (0.28991) | -1 | -1 |
| G: -5683.64846 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.89725 HOMO: -7.17020 LUMO: -1.02043 factor:1 | -1 (0.11690) | -1 | -1 |
| G: -5683.64846 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.72764 HOMO: -6.26406 LUMO: -0.96328 factor:1 | -1 (0.28651) | -1 | -1 |
| G: -5683.64846 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.82490 HOMO: -6.50896 LUMO: -0.38640 factor:1 | -1 (0.18926) | -1 | -1 |
| G: -5683.64846 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.06809 HOMO: -7.27632 LUMO: -1.17553 factor:1 | 1 (-2.05394) | -1 | -1 |
| G: -5683.64846 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.73222 HOMO: -6.54162 LUMO: -1.36873 factor:1 | 1 (-1.71807) | -1 | -1 |
| G: -5683.64846 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.72439 HOMO: -6.42733 LUMO: -1.15648 factor:1 | 1 (-1.71024) | -1 | -1 |
| G: -5683.64846 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.80929 HOMO: -6.73754 LUMO: -2.58780 factor:1 | 1 (-1.79514) | -1 | -1 |
| G: -5683.64846 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.15213 HOMO: -7.20285 LUMO: 0.75103 factor:1 | 1 (-1.13798) | 1 | 1 |
| G: -5683.64846 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.02149 HOMO: -6.98788 LUMO: 0.34831 factor:1 | 1 (-1.00734) | -1 | -1 |
| G: -5683.64846 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.77592 HOMO: -6.80013 LUMO: -1.11567 factor:1 | -1 (0.23824) | -1 | -1 |
| G: -5683.64846 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.07168 HOMO: -6.67767 LUMO: -0.82450 factor:1 | 1 (-0.05752) | -1 | -1 |
| G: -5683.64846 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.38023 HOMO: -6.84911 LUMO: -0.21497 factor:1 | 1 (-0.36607) | -1 | -1 |
| G: -5683.64846 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.04496 HOMO: -6.23141 LUMO: 0.21769 factor:1 | 1 (-0.03080) | -1 | -1 |
| G: -5683.64846 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.71022 HOMO: -6.68312 LUMO: 0.16327 factor:1 | 1 (-0.69607) | -1 | -1 |
| G: -5683.64846 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.87219 HOMO: -7.04503 LUMO: -1.04220 factor:1 | -1 (0.14196) | -1 | -1 |
| G: -5683.64846 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.94520 HOMO: -6.67495 LUMO: -0.71294 factor:1 | -1 (0.06895) | -1 | -1 |
| G: -5683.64846 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.96631 HOMO: -6.70216 LUMO: -0.55239 factor:1 | -1 (0.04784) | -1 | -1 |
| G: -5683.64846 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.00319 HOMO: -6.60420 LUMO: -0.71294 factor:1 | -1 (0.01097) | -1 | -1 |
| G: -5683.64846 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.69409 HOMO: -7.40694 LUMO: 0.11973 factor:1 | -1 (0.32006) | 1 | 1 |
| G: -5683.64846 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.23133 HOMO: -6.58788 LUMO: -0.29116 factor:1 | 1 (-0.21717) | -1 | -1 |
| G: -5683.64846 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.02832 HOMO: -6.63686 LUMO: -0.32654 factor:1 | 1 (-1.01417) | -1 | -1 |
| G: -5683.64846 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.90209 HOMO: -6.85183 LUMO: -0.95512 factor:1 | 1 (-0.88793) | -1 | -1 |
| G: -5683.64846 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.24544 HOMO: -6.82189 LUMO: -0.88165 factor:1 | 1 (-1.23129) | -1 | -1 |
| G: -5683.64846 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.59351 HOMO: -6.97428 LUMO: -1.03947 factor:1 | 1 (-0.57936) | -1 | -1 |
| G: -5683.64846 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.19858 HOMO: -6.51441 LUMO: -0.05714 factor:1 | 1 (-1.18443) | -1 | -1 |
| G: -5683.64846 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.08071 HOMO: -6.61509 LUMO: -0.77008 factor:1 | 1 (-0.06656) | -1 | -1 |
| G: -5683.64846 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.42820 HOMO: -7.36340 LUMO: 0.29116 factor:1 | 1 (-0.41405) | 1 | 1 |
| G: -5683.64846 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.20775 HOMO: -6.64230 LUMO: -0.79185 factor:1 | 1 (-1.19360) | -1 | -1 |
| G: -5683.64846 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.61147 HOMO: -6.56883 LUMO: -1.03403 factor:1 | 1 (-0.59732) | -1 | -1 |
| G: -5683.64846 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11945.15179 HOMO: -6.69400 LUMO: -0.77825 factor:1 | -1 (2.86237) | -1 | -1 |
| G: -5683.64846 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11944.10385 HOMO: -6.37019 LUMO: -0.79185 factor:1 | -1 (3.91030) | -1 | -1 |
| G: -5683.64846 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11944.66465 HOMO: -6.49808 LUMO: -0.94424 factor:1 | -1 (3.34950) | -1 | -1 |
| G: -5683.64846 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.22189 HOMO: -6.91713 LUMO: -0.75376 factor:1 | -1 (0.79226) | -1 | -1 |
| G: -5683.64846 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11946.21766 HOMO: -7.13755 LUMO: 0.41361 factor:1 | -1 (1.79650) | 1 | 1 |
| G: -5683.64846 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11946.15066 HOMO: -7.12122 LUMO: 0.39457 factor:1 | -1 (1.86349) | 1 | 1 |
| G: -5683.64846 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11945.03606 HOMO: -6.59332 LUMO: -0.57144 factor:1 | -1 (2.97810) | -1 | -1 |
| G: -5683.64846 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11945.07929 HOMO: -6.62325 LUMO: -0.66940 factor:1 | -1 (2.93486) | -1 | -1 |
| G: -5683.64846 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11946.83174 HOMO: -6.90897 LUMO: -0.08708 factor:1 | -1 (1.18242) | -1 | -1 |
| G: -5683.64846 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11946.73973 HOMO: -6.65591 LUMO: -0.81090 factor:1 | -1 (1.27442) | -1 | -1 |
| G: -5683.64846 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.32050 HOMO: -6.65318 LUMO: -0.94696 factor:1 | 1 (-0.30635) | -1 | -1 |
| G: -5683.64846 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.32597 HOMO: -6.96067 LUMO: -1.03675 factor:1 | 1 (-0.31182) | -1 | -1 |
| G: -5683.64846 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.65245 HOMO: -6.23141 LUMO: -0.66396 factor:1 | 1 (-0.63830) | -1 | -1 |
| G: -5683.64846 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.77833 HOMO: -6.52529 LUMO: -0.78369 factor:1 | 1 (-0.76418) | -1 | -1 |
| G: -5683.64846 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.27352 HOMO: -6.39468 LUMO: -0.40817 factor:1 | 1 (-1.25937) | -1 | -1 |
| G: -5683.64846 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.61351 HOMO: -6.76203 LUMO: -0.20409 factor:1 | 1 (-0.59936) | -1 | -1 |
| G: -5683.64846 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.27927 HOMO: -6.96611 LUMO: -0.90342 factor:1 | 1 (-0.26512) | -1 | -1 |
| G: -5683.64846 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.13564 HOMO: -6.54706 LUMO: -0.87893 factor:1 | 1 (-1.12149) | -1 | -1 |
| G: -5683.64846 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.56328 HOMO: -7.24367 LUMO: -0.97689 factor:1 | 1 (-0.54913) | -1 | -1 |
| G: -5683.64846 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.11989 HOMO: -6.61781 LUMO: 1.43404 factor:1 | 1 (-1.10573) | -1 | -1 |
| G: -5683.64846 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.63215 HOMO: -6.17971 LUMO: 1.79867 factor:1 | 1 (-0.61800) | -1 | -1 |
| G: -5683.64846 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.04961 HOMO: -5.73344 LUMO: 2.13609 factor:1 | 1 (-0.03546) | -1 | -1 |
| G: -5683.64846 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.02097 HOMO: -6.72121 LUMO: 2.06807 factor:1 | 1 (-1.00682) | -1 | -1 |
| G: -5683.64846 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.92272 HOMO: -6.91169 LUMO: 2.02997 factor:1 | -1 (0.09143) | -1 | -1 |
| G: -5683.64846 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.10089 HOMO: -7.06408 LUMO: 1.41499 factor:1 | 1 (-1.08674) | 1 | 1 |
| G: -5683.64846 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.57101 HOMO: -6.94162 LUMO: -0.90070 factor:1 | 1 (-0.55685) | -1 | -1 |
| G: -5683.64846 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11946.62022 HOMO: -7.09401 LUMO: 0.35103 factor:1 | -1 (1.39393) | 1 | 1 |
| G: -5683.64846 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.01072 HOMO: -6.78652 LUMO: 0.91974 factor:1 | -1 (0.00343) | -1 | -1 |
| G: -5683.64846 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.32216 HOMO: -6.32937 LUMO: -1.89119 factor:1 | 1 (-0.30801) | -1 | -1 |
| G: -5683.64846 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.61306 HOMO: -7.12666 LUMO: -1.06397 factor:1 | -1 (0.40110) | -1 | -1 |
| G: -5683.64846 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.80860 HOMO: -6.38107 LUMO: -1.43132 factor:1 | -1 (0.20555) | -1 | -1 |
| G: -5683.64846 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.98784 HOMO: -7.09129 LUMO: 0.08980 factor:1 | -1 (0.02631) | 1 | 1 |
| G: -5683.64846 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.69631 HOMO: -6.31304 LUMO: -0.57960 factor:1 | 1 (-0.68216) | -1 | -1 |
| G: -5683.64846 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.74949 HOMO: -6.94435 LUMO: -0.74287 factor:1 | -1 (0.26466) | -1 | -1 |
| G: -5683.64846 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.46725 HOMO: -6.35658 LUMO: -1.53472 factor:1 | 1 (-0.45310) | -1 | -1 |
| G: -5683.64846 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.56927 HOMO: -6.39740 LUMO: -1.48846 factor:1 | -1 (0.44488) | -1 | -1 |
| G: -5683.64846 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.00953 HOMO: -7.05319 LUMO: -0.33198 factor:1 | -1 (0.00463) | -1 | -1 |
| G: -5683.64846 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.75109 HOMO: -6.68040 LUMO: -0.09252 factor:1 | 1 (-0.73694) | -1 | -1 |
| G: -5683.64846 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.91638 HOMO: -6.35930 LUMO: -0.43266 factor:1 | -1 (0.09777) | -1 | -1 |
| G: -5683.64846 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.51896 HOMO: -6.59604 LUMO: -1.45853 factor:1 | -1 (0.49519) | -1 | -1 |
| G: -5683.64846 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.62995 HOMO: -6.46270 LUMO: -1.49391 factor:1 | -1 (0.38420) | -1 | -1 |
| G: -5683.64846 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.56450 HOMO: -7.05863 LUMO: -1.04764 factor:1 | 1 (-0.55035) | -1 | -1 |
| G: -5683.64846 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.47495 HOMO: -7.14027 LUMO: -0.81634 factor:1 | 1 (-0.46080) | -1 | -1 |
| G: -5683.64846 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.91245 HOMO: -6.80285 LUMO: -0.74287 factor:1 | 1 (-0.89830) | -1 | -1 |
| G: -5683.64846 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.07099 HOMO: -6.53890 LUMO: -1.13471 factor:1 | 1 (-1.05684) | -1 | -1 |
| G: -5683.64846 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.95538 HOMO: -6.49808 LUMO: -1.35513 factor:1 | -1 (0.05878) | -1 | -1 |
| G: -5683.64846 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.83867 HOMO: -6.75931 LUMO: -1.49663 factor:1 | -1 (0.17549) | -1 | -1 |
| G: -5683.64846 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.72329 HOMO: -6.84638 LUMO: -0.77552 factor:1 | -1 (0.29086) | -1 | -1 |
| G: -5683.64846 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11946.61565 HOMO: -6.65863 LUMO: -1.34696 factor:1 | -1 (1.39850) | -1 | -1 |
| G: -5683.64846 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.13772 HOMO: -6.25590 LUMO: -2.36467 factor:1 | 1 (-0.12357) | -1 | -1 |
| G: -5683.64846 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.50352 HOMO: -7.24911 LUMO: 0.33470 factor:1 | 1 (-0.48937) | 1 | 1 |
| G: -5683.64846 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.87969 HOMO: -6.65863 LUMO: -0.75648 factor:1 | 1 (-0.86554) | -1 | -1 |
| G: -5683.64846 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.89365 HOMO: -6.31576 LUMO: -0.83267 factor:1 | 1 (-0.87950) | -1 | -1 |
| G: -5683.64846 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.64393 HOMO: -6.64774 LUMO: -0.66124 factor:1 | 1 (-0.62978) | -1 | -1 |
| G: -5683.64846 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.96631 HOMO: -6.75387 LUMO: -1.00138 factor:1 | 1 (-0.95215) | -1 | -1 |
| G: -5683.64846 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11946.79141 HOMO: -6.52529 LUMO: -0.68301 factor:1 | -1 (1.22274) | -1 | -1 |
| G: -5683.64846 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.82537 HOMO: -6.59332 LUMO: -0.68028 factor:1 | 1 (-1.81122) | -1 | -1 |
| G: -5683.64846 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.53630 HOMO: -5.98650 LUMO: 0.31565 factor:1 | 1 (-1.52215) | -1 | -1 |
| G: -5683.64846 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.81604 HOMO: -6.59876 LUMO: 0.22585 factor:1 | 1 (-0.80189) | -1 | -1 |
| G: -5683.64846 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.76920 HOMO: -6.72121 LUMO: 0.10340 factor:1 | 1 (-1.75505) | -1 | -1 |
| G: -5683.64846 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.01159 HOMO: -6.09807 LUMO: 0.20136 factor:1 | 1 (-0.99743) | -1 | -1 |
| G: -5683.64846 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.84897 HOMO: -6.31576 LUMO: 0.06259 factor:1 | 1 (-0.83482) | -1 | -1 |
| G: -5683.64846 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.49641 HOMO: -6.35658 LUMO: -0.58232 factor:1 | 1 (-1.48226) | -1 | -1 |
| G: -5683.64846 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.87323 HOMO: -6.34842 LUMO: -0.55783 factor:1 | 1 (-1.85908) | -1 | -1 |
| G: -5683.64846 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.13502 HOMO: -6.47359 LUMO: -0.57144 factor:1 | 1 (-1.12086) | -1 | -1 |
| G: -5683.64846 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.99654 HOMO: -6.42189 LUMO: -0.09796 factor:1 | 1 (-0.98239) | -1 | -1 |
| G: -5683.64846 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.55497 HOMO: -6.35658 LUMO: -0.31293 factor:1 | 1 (-1.54082) | -1 | -1 |
| G: -5683.64846 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.70016 HOMO: -7.35524 LUMO: 0.10340 factor:1 | -1 (0.31399) | 1 | 1 |
| G: -5683.64846 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.68176 HOMO: -7.10217 LUMO: 0.36463 factor:1 | -1 (0.33239) | 1 | 1 |
| G: -5683.64846 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.30611 HOMO: -6.43549 LUMO: -0.56872 factor:1 | -1 (0.70804) | -1 | -1 |
| G: -5683.64846 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.24539 HOMO: -6.50080 LUMO: -0.71294 factor:1 | 1 (-0.23124) | -1 | -1 |
| G: -5683.64846 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.26772 HOMO: -6.59060 LUMO: -0.57960 factor:1 | -1 (0.74644) | -1 | -1 |
| G: -5683.64846 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.07315 HOMO: -6.78924 LUMO: -0.31565 factor:1 | -1 (0.94100) | -1 | -1 |
| G: -5683.64846 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.21280 HOMO: -6.35658 LUMO: 0.07891 factor:1 | -1 (0.80135) | -1 | -1 |
| G: -5683.64846 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.16540 HOMO: -6.74026 LUMO: -0.87621 factor:1 | -1 (0.84875) | -1 | -1 |
| G: -5683.64846 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.16807 HOMO: -6.54434 LUMO: 0.81906 factor:1 | -1 (0.84608) | -1 | -1 |
| G: -5683.64846 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11946.87361 HOMO: -6.66135 LUMO: 1.40955 factor:1 | -1 (1.14054) | -1 | -1 |
| G: -5683.64846 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11946.62610 HOMO: -6.73754 LUMO: -2.54971 factor:1 | -1 (1.38805) | -1 | -1 |
| G: -5683.64846 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11946.86474 HOMO: -6.65318 LUMO: 0.69389 factor:1 | -1 (1.14941) | -1 | -1 |
| G: -5683.64846 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11946.58125 HOMO: -6.73482 LUMO: 0.62858 factor:1 | -1 (1.43290) | -1 | -1 |
| G: -5683.64846 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.62650 HOMO: -6.83550 LUMO: 0.68573 factor:1 | -1 (0.38765) | -1 | -1 |
| G: -5683.64846 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.14547 HOMO: -6.83278 LUMO: 0.45987 factor:1 | 1 (-0.13132) | -1 | -1 |
| G: -5683.64846 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11946.60939 HOMO: -6.78380 LUMO: 0.68301 factor:1 | -1 (1.40476) | -1 | -1 |
| G: -5683.64846 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.32718 HOMO: -6.90625 LUMO: 1.36601 factor:1 | 1 (-1.31303) | -1 | -1 |
| G: -5683.64846 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.19045 HOMO: -6.82734 LUMO: 1.48302 factor:1 | 1 (-1.17629) | -1 | -1 |
| G: -5683.64846 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.84832 HOMO: -6.44094 LUMO: -0.94424 factor:1 | 1 (-0.83417) | -1 | -1 |
| G: -5683.64846 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.18027 HOMO: -6.91441 LUMO: 0.28844 factor:1 | 1 (-1.16612) | -1 | -1 |
| G: -5683.64846 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.54962 HOMO: -6.49808 LUMO: -0.51157 factor:1 | 1 (-0.53547) | -1 | -1 |
| G: -5683.64846 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.21552 HOMO: -7.09673 LUMO: -0.06259 factor:1 | 1 (-0.20136) | 1 | 1 |
| G: -5683.64846 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.24468 HOMO: -6.77019 LUMO: 0.92247 factor:1 | 1 (-1.23053) | -1 | -1 |
| G: -5683.64846 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.65471 HOMO: -6.75931 LUMO: 1.13744 factor:1 | 1 (-0.64056) | -1 | -1 |
| G: -5683.64846 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.29962 HOMO: -6.15794 LUMO: 1.12383 factor:1 | 1 (-1.28547) | -1 | -1 |
| G: -5683.64846 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.82679 HOMO: -6.59604 LUMO: 1.19458 factor:1 | 1 (-0.81264) | -1 | -1 |
| G: -5683.64846 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.77783 HOMO: -7.09401 LUMO: 0.60137 factor:1 | 1 (-1.76368) | 1 | 1 |
| G: -5683.64846 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.18846 HOMO: -6.34025 LUMO: 0.48164 factor:1 | 1 (-1.17431) | -1 | -1 |
| G: -5683.64846 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.86951 HOMO: -6.72665 LUMO: -2.47624 factor:1 | 1 (-1.85535) | -1 | -1 |
| G: -5683.64846 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.71271 HOMO: -6.48175 LUMO: 0.58232 factor:1 | 1 (-1.69856) | -1 | -1 |
| G: -5683.64846 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.83893 HOMO: -6.94162 LUMO: 0.28300 factor:1 | 1 (-0.82478) | -1 | -1 |
| G: -5683.64846 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.92771 HOMO: -6.65591 LUMO: 0.57144 factor:1 | 1 (-1.91356) | -1 | -1 |
| G: -5683.64846 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.34588 HOMO: -6.58788 LUMO: -1.03947 factor:1 | 1 (-1.33173) | -1 | -1 |
| G: -5683.64846 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.32927 HOMO: -7.18108 LUMO: 0.37824 factor:1 | 1 (-2.31512) | 1 | 1 |
| G: -5683.64846 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.48294 HOMO: -6.63958 LUMO: -1.52112 factor:1 | 1 (-1.46879) | -1 | -1 |
| G: -5683.64846 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.34856 HOMO: -6.12528 LUMO: -0.53606 factor:1 | 1 (-2.33441) | -1 | -1 |
| G: -5683.64846 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.84485 HOMO: -6.22324 LUMO: -0.87893 factor:1 | 1 (-1.83070) | -1 | -1 |
| G: -5683.64846 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.31502 HOMO: -6.62053 LUMO: -0.91974 factor:1 | 1 (-1.30087) | -1 | -1 |
| G: -5683.64846 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.03767 HOMO: -6.84366 LUMO: -0.83811 factor:1 | 1 (-2.02352) | -1 | -1 |
| G: -5683.64846 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.62994 HOMO: -7.26000 LUMO: 0.25851 factor:1 | 1 (-1.61578) | 1 | 1 |
| G: -5683.64846 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.15885 HOMO: -6.49536 LUMO: -0.63403 factor:1 | 1 (-1.14470) | -1 | -1 |
| G: -5683.64846 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.01511 HOMO: -6.45726 LUMO: -0.77825 factor:1 | 1 (-2.00096) | -1 | -1 |
| G: -5683.64846 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.94643 HOMO: -6.74570 LUMO: -0.75103 factor:1 | 1 (-1.93228) | -1 | -1 |
| G: -5683.64846 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.24612 HOMO: -7.20285 LUMO: 0.10612 factor:1 | 1 (-1.23197) | 1 | 1 |
| G: -5683.64846 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.89205 HOMO: -6.45182 LUMO: -0.56600 factor:1 | 1 (-0.87789) | -1 | -1 |
| G: -5683.64846 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.21249 HOMO: -6.83278 LUMO: -0.71838 factor:1 | 1 (-1.19834) | -1 | -1 |
| G: -5683.64846 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.33655 HOMO: -7.01510 LUMO: -1.09662 factor:1 | 1 (-0.32240) | -1 | -1 |
| G: -5683.64846 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.89188 HOMO: -6.48719 LUMO: 0.16871 factor:1 | 1 (-0.87773) | -1 | -1 |
| G: -5683.64846 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.45807 HOMO: -7.30898 LUMO: 0.26667 factor:1 | 1 (-1.44392) | 1 | 1 |
| G: -5683.64846 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.70238 HOMO: -6.68856 LUMO: -0.78641 factor:1 | 1 (-0.68823) | -1 | -1 |
| G: -5683.64846 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.60658 HOMO: -6.56883 LUMO: -1.00682 factor:1 | -1 (0.40757) | -1 | -1 |
| G: -5683.64846 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.73313 HOMO: -6.41100 LUMO: -0.48980 factor:1 | 1 (-0.71898) | -1 | -1 |
| G: -5683.64846 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.68228 HOMO: -6.52257 LUMO: -0.59865 factor:1 | -1 (0.33187) | -1 | -1 |
| G: -5683.64846 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.83286 HOMO: -6.63686 LUMO: -0.56055 factor:1 | 1 (-0.81871) | -1 | -1 |
| G: -5683.64846 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.00773 HOMO: -6.79740 LUMO: -0.75376 factor:1 | -1 (0.00642) | -1 | -1 |
| G: -5683.64846 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11945.11470 HOMO: -5.89127 LUMO: 0.22313 factor:1 | -1 (2.89945) | -1 | -1 |
| G: -5683.64846 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11945.18147 HOMO: -6.34842 LUMO: 0.11429 factor:1 | -1 (2.83268) | -1 | -1 |
| G: -5683.64846 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11944.66293 HOMO: -6.13617 LUMO: 1.94834 factor:1 | -1 (3.35122) | -1 | -1 |
| G: -5683.64846 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.26749 HOMO: -6.50080 LUMO: 1.74153 factor:1 | 1 (-0.25334) | -1 | -1 |
| G: -5683.64846 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.45307 HOMO: -6.33481 LUMO: 1.68438 factor:1 | 1 (-0.43892) | -1 | -1 |
| G: -5683.64846 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.17706 HOMO: -6.53073 LUMO: 1.95106 factor:1 | 1 (-1.16291) | -1 | -1 |
| G: -5683.64846 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.46799 HOMO: -6.46270 LUMO: 1.89935 factor:1 | -1 (0.54616) | -1 | -1 |
| G: -5683.64846 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.95205 HOMO: -5.87222 LUMO: 1.91568 factor:1 | 1 (-0.93789) | -1 | -1 |
| G: -5683.64846 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.85019 HOMO: -6.07630 LUMO: 1.81500 factor:1 | 1 (-0.83604) | -1 | -1 |
| G: -5683.64846 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.19757 HOMO: -6.20964 LUMO: 1.81500 factor:1 | 1 (-1.18342) | -1 | -1 |
| G: -5683.64846 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.14813 HOMO: -6.15522 LUMO: 1.90752 factor:1 | 1 (-1.13398) | -1 | -1 |
| G: -5683.64846 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11946.99155 HOMO: -6.11984 LUMO: 1.95378 factor:1 | -1 (1.02260) | -1 | -1 |
| G: -5683.64846 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.03313 HOMO: -6.58516 LUMO: 2.04358 factor:1 | -1 (0.98102) | -1 | -1 |
| G: -5683.64846 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11946.82847 HOMO: -7.37156 LUMO: 0.24490 factor:1 | -1 (1.18568) | 1 | 1 |
| G: -5683.64846 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.51598 HOMO: -6.36474 LUMO: -0.90070 factor:1 | 1 (-0.50183) | -1 | -1 |
| G: -5683.64846 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.62707 HOMO: -6.43549 LUMO: -0.40817 factor:1 | -1 (0.38708) | -1 | -1 |
| G: -5683.64846 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.86130 HOMO: -7.32258 LUMO: 0.29388 factor:1 | 1 (-0.84714) | 1 | 1 |
| G: -5683.64846 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.92098 HOMO: -6.41372 LUMO: -0.20409 factor:1 | -1 (0.09317) | -1 | -1 |
| G: -5683.64846 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.97595 HOMO: -7.18381 LUMO: 0.42722 factor:1 | -1 (0.03820) | 1 | 1 |
| G: -5683.64846 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.83189 HOMO: -6.53890 LUMO: -0.54151 factor:1 | -1 (0.18226) | -1 | -1 |
| G: -5683.64846 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.70548 HOMO: -6.61509 LUMO: 0.08708 factor:1 | 1 (-1.69132) | -1 | -1 |
| G: -5683.64846 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.79614 HOMO: -6.78108 LUMO: 2.03541 factor:1 | 1 (-1.78199) | -1 | -1 |
| G: -5683.64846 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.89193 HOMO: -6.50896 LUMO: 1.53472 factor:1 | 1 (-1.87778) | -1 | -1 |
| G: -5683.64846 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.42966 HOMO: -6.65591 LUMO: 1.80411 factor:1 | 1 (-1.41551) | -1 | -1 |
| G: -5683.64846 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.72466 HOMO: -6.64502 LUMO: 1.52112 factor:1 | 1 (-1.71051) | -1 | -1 |
| G: -5683.64846 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.17433 HOMO: -6.72938 LUMO: 1.48030 factor:1 | 1 (-2.16018) | -1 | -1 |
| G: -5683.64846 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.14122 HOMO: -6.16882 LUMO: 1.96466 factor:1 | 1 (-1.12707) | -1 | -1 |
| G: -5683.64846 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.10153 HOMO: -6.22597 LUMO: 1.43132 factor:1 | 1 (-0.08738) | -1 | -1 |
| G: -5683.64846 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.06283 HOMO: -6.57699 LUMO: 2.05718 factor:1 | 1 (-0.04868) | -1 | -1 |
| G: -5683.64846 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.12526 HOMO: -6.52529 LUMO: 1.89663 factor:1 | -1 (0.88889) | -1 | -1 |
| G: -5683.64846 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.92655 HOMO: -6.30760 LUMO: 1.88031 factor:1 | 1 (-0.91240) | -1 | -1 |
| G: -5683.64846 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.89649 HOMO: -6.14977 LUMO: 1.92657 factor:1 | -1 (0.11766) | -1 | -1 |
| G: -5683.64846 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.73135 HOMO: -6.20964 LUMO: 1.83949 factor:1 | 1 (-1.71720) | -1 | -1 |
| G: -5683.64846 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.41676 HOMO: -6.31848 LUMO: 1.91296 factor:1 | 1 (-1.40261) | -1 | -1 |
| G: -5683.64846 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.71274 HOMO: -5.80691 LUMO: 2.19868 factor:1 | 1 (-1.69859) | -1 | -1 |
| G: -5683.64846 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.01174 HOMO: -6.00827 LUMO: 2.15514 factor:1 | 1 (-1.99759) | -1 | -1 |
| G: -5683.64846 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.07052 HOMO: -6.51713 LUMO: 2.08711 factor:1 | 1 (-2.05636) | -1 | -1 |
| G: -5683.64846 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.50689 HOMO: -6.32937 LUMO: 2.11705 factor:1 | 1 (-1.49274) | -1 | -1 |
| G: -5683.64846 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.24987 HOMO: -6.26678 LUMO: 1.95922 factor:1 | 1 (-2.23571) | -1 | -1 |
| G: -5683.64846 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.70651 HOMO: -6.43005 LUMO: 2.56603 factor:1 | 1 (-1.69236) | -1 | -1 |
| G: -5683.64846 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.48074 HOMO: -6.41644 LUMO: 2.68304 factor:1 | 1 (-1.46658) | -1 | -1 |
| G: -5683.64846 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.54000 HOMO: -5.97834 LUMO: 2.02997 factor:1 | 1 (-1.52585) | -1 | -1 |
| G: -5683.64846 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.97746 HOMO: -6.14161 LUMO: 1.77690 factor:1 | 1 (-0.96331) | -1 | -1 |
| G: -5683.64846 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.14356 HOMO: -6.21508 LUMO: 1.80411 factor:1 | 1 (-1.12941) | -1 | -1 |
| G: -5683.64846 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.95939 HOMO: -6.46270 LUMO: 2.34562 factor:1 | 1 (-0.94524) | -1 | -1 |
| G: -5683.64846 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.83938 HOMO: -6.39195 LUMO: -0.75920 factor:1 | 1 (-1.82523) | -1 | -1 |
| G: -5683.64846 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.85209 HOMO: -7.08584 LUMO: -1.14016 factor:1 | 1 (-1.83794) | -1 | -1 |
| G: -5683.64846 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.59762 HOMO: -6.70216 LUMO: -0.65035 factor:1 | 1 (-0.58347) | -1 | -1 |
| G: -5683.64846 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.10459 HOMO: -6.79468 LUMO: -0.83811 factor:1 | 1 (-1.09044) | -1 | -1 |
| G: -5683.64846 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.74486 HOMO: -6.99877 LUMO: -0.79729 factor:1 | 1 (-0.73071) | -1 | -1 |
| G: -5683.64846 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.68213 HOMO: -7.08040 LUMO: -0.85444 factor:1 | 1 (-1.66798) | -1 | -1 |
| G: -5683.64846 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.49932 HOMO: -7.39333 LUMO: 0.12789 factor:1 | 1 (-1.48517) | 1 | 1 |
| G: -5683.64846 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.03191 HOMO: -7.05047 LUMO: 0.13878 factor:1 | 1 (-1.01776) | -1 | -1 |
| G: -5683.64846 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.68308 HOMO: -6.90897 LUMO: -0.77552 factor:1 | 1 (-1.66893) | -1 | -1 |
| G: -5683.64846 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.33586 HOMO: -7.25456 LUMO: 0.05170 factor:1 | 1 (-1.32171) | 1 | 1 |
| G: -5683.64846 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.14046 HOMO: -6.84638 LUMO: -0.84355 factor:1 | 1 (-1.12631) | -1 | -1 |
| G: -5683.64846 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.67520 HOMO: -6.78108 LUMO: -0.81634 factor:1 | 1 (-0.66105) | -1 | -1 |
| G: -5683.64846 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.24609 HOMO: -6.74570 LUMO: -0.77280 factor:1 | 1 (-1.23194) | -1 | -1 |
| G: -5683.64846 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.07006 HOMO: -7.28177 LUMO: -1.68438 factor:1 | 1 (-1.05591) | -1 | -1 |
| G: -5683.64846 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.77226 HOMO: -7.22190 LUMO: -1.63540 factor:1 | 1 (-0.75811) | -1 | -1 |
| G: -5683.64846 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.90585 HOMO: -7.15932 LUMO: -1.57554 factor:1 | -1 (0.10830) | -1 | -1 |
| G: -5683.64846 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.92240 HOMO: -6.57971 LUMO: -0.93063 factor:1 | -1 (0.09176) | -1 | -1 |
| G: -5683.64846 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.59716 HOMO: -6.88176 LUMO: 0.58232 factor:1 | -1 (0.41699) | -1 | -1 |
| G: -5683.64846 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.45898 HOMO: -6.85727 LUMO: 0.51430 factor:1 | 1 (-0.44482) | -1 | -1 |
| G: -5683.64846 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.61661 HOMO: -6.83550 LUMO: 0.87893 factor:1 | 1 (-0.60246) | -1 | -1 |
| G: -5683.64846 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.84062 HOMO: -7.06680 LUMO: 0.87621 factor:1 | 1 (-0.82646) | 1 | 1 |
| G: -5683.64846 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.58880 HOMO: -6.52257 LUMO: 0.81362 factor:1 | 1 (-0.57465) | -1 | -1 |
| G: -5683.64846 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.78958 HOMO: -6.95523 LUMO: 1.17009 factor:1 | -1 (0.22458) | -1 | -1 |
| G: -5683.64846 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.79328 HOMO: -7.21374 LUMO: 0.97145 factor:1 | -1 (0.22087) | 1 | 1 |
| G: -5683.64846 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.44201 HOMO: -6.81373 LUMO: -1.54561 factor:1 | -1 (0.57215) | -1 | -1 |
| G: -5683.64846 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.32939 HOMO: -6.86543 LUMO: -1.52656 factor:1 | 1 (-1.31524) | -1 | -1 |
| G: -5683.64846 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.57494 HOMO: -6.90081 LUMO: -0.78097 factor:1 | 1 (-1.56079) | -1 | -1 |
| G: -5683.64846 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.72785 HOMO: -6.64502 LUMO: -0.82723 factor:1 | 1 (-0.71370) | -1 | -1 |
| G: -5683.64846 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.74978 HOMO: -6.65591 LUMO: -0.82178 factor:1 | 1 (-1.73562) | -1 | -1 |
| G: -5683.64846 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.68801 HOMO: -6.79468 LUMO: -1.46397 factor:1 | 1 (-1.67385) | -1 | -1 |
| G: -5683.64846 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.51451 HOMO: -7.25728 LUMO: 0.73743 factor:1 | 1 (-1.50035) | 1 | -1 |
| G: -5683.64846 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.88757 HOMO: -7.00149 LUMO: 1.30070 factor:1 | 1 (-1.87342) | -1 | -1 |
| G: -5683.64846 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.02114 HOMO: -7.07768 LUMO: 0.78097 factor:1 | 1 (-1.00698) | 1 | -1 |
| G: -5683.64846 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.79702 HOMO: -6.86271 LUMO: 0.86260 factor:1 | 1 (-0.78287) | -1 | -1 |
| G: -5683.64846 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.15809 HOMO: -6.94707 LUMO: 0.39729 factor:1 | 1 (-1.14394) | -1 | -1 |
| G: -5683.64846 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.82078 HOMO: -6.79740 LUMO: 0.67484 factor:1 | 1 (-0.80663) | -1 | -1 |
| G: -5683.64846 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.46162 HOMO: -6.91986 LUMO: -1.14288 factor:1 | -1 (0.55253) | -1 | -1 |
| G: -5683.64846 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11946.66011 HOMO: -6.31576 LUMO: 1.01771 factor:1 | -1 (1.35404) | -1 | -1 |
| G: -5683.64846 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.99105 HOMO: -6.81645 LUMO: 0.81362 factor:1 | -1 (0.02310) | -1 | -1 |
| G: -5683.64846 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.07283 HOMO: -6.92258 LUMO: -0.99594 factor:1 | -1 (0.94132) | -1 | -1 |
| G: -5683.64846 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.36987 HOMO: -6.81373 LUMO: 0.61770 factor:1 | -1 (0.64428) | -1 | -1 |
| G: -5683.64846 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.64582 HOMO: -7.18653 LUMO: 1.19186 factor:1 | -1 (0.36833) | 1 | 1 |
| G: -5683.64846 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.73940 HOMO: -7.00693 LUMO: 0.45715 factor:1 | -1 (0.27475) | -1 | -1 |
| G: -5683.64846 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.45066 HOMO: -7.11306 LUMO: 0.53334 factor:1 | -1 (0.56349) | 1 | 1 |
| G: -5683.64846 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.85347 HOMO: -6.63414 LUMO: -1.64357 factor:1 | -1 (0.16068) | -1 | -1 |
| G: -5683.64846 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11946.89729 HOMO: -6.22052 LUMO: -0.74015 factor:1 | -1 (1.11686) | -1 | -1 |
| G: -5683.64846 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11946.96104 HOMO: -6.81101 LUMO: -0.50069 factor:1 | -1 (1.05311) | -1 | -1 |
| G: -5683.64846 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11946.65766 HOMO: -6.71849 LUMO: -0.51974 factor:1 | -1 (1.35649) | -1 | -1 |
| G: -5683.64846 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.02606 HOMO: -6.72121 LUMO: -1.77690 factor:1 | 1 (-1.01191) | -1 | -1 |
| G: -5683.64846 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.94869 HOMO: -6.94162 LUMO: -1.78779 factor:1 | 1 (-1.93454) | -1 | -1 |
| G: -5683.64846 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.69802 HOMO: -6.91169 LUMO: 0.88981 factor:1 | 1 (-1.68387) | -1 | -1 |
| G: -5683.64846 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.91142 HOMO: -6.97428 LUMO: 0.70750 factor:1 | 1 (-0.89727) | -1 | -1 |
| G: -5683.64846 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.91161 HOMO: -6.74842 LUMO: 1.15921 factor:1 | 1 (-0.89746) | -1 | -1 |
| G: -5683.64846 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.85128 HOMO: -7.25183 LUMO: -0.99594 factor:1 | 1 (-0.83713) | -1 | -1 |
| G: -5683.64846 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.92496 HOMO: -6.43821 LUMO: -1.00410 factor:1 | 1 (-1.91081) | -1 | -1 |
| G: -5683.64846 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.93402 HOMO: -6.52257 LUMO: -0.68573 factor:1 | 1 (-1.91987) | -1 | -1 |
| G: -5683.64846 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.20756 HOMO: -6.60148 LUMO: -0.52518 factor:1 | 1 (-1.19341) | -1 | -1 |
| G: -5683.64846 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.38686 HOMO: -6.07086 LUMO: -1.39594 factor:1 | 1 (-1.37271) | -1 | -1 |
| G: -5683.64846 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.60815 HOMO: -6.78108 LUMO: -1.54833 factor:1 | 1 (-0.59400) | -1 | -1 |
| G: -5683.64846 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.97119 HOMO: -6.73482 LUMO: -1.01498 factor:1 | 1 (-1.95704) | -1 | -1 |
| G: -5683.64846 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.27336 HOMO: -6.85183 LUMO: 1.06669 factor:1 | 1 (-1.25921) | -1 | -1 |
| G: -5683.64846 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.99289 HOMO: -6.98516 LUMO: 1.43948 factor:1 | 1 (-0.97874) | -1 | -1 |
| G: -5683.64846 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.90633 HOMO: -6.94162 LUMO: 0.79185 factor:1 | 1 (-0.89218) | -1 | -1 |
| G: -5683.64846 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.95791 HOMO: -6.67495 LUMO: -1.06669 factor:1 | -1 (0.05625) | -1 | -1 |
| G: -5683.64846 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.02365 HOMO: -6.88720 LUMO: -1.00682 factor:1 | 1 (-0.00950) | -1 | -1 |
| G: -5683.64846 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.54353 HOMO: -6.85999 LUMO: -0.78097 factor:1 | -1 (0.47062) | -1 | -1 |
| G: -5683.64846 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.79880 HOMO: -6.51713 LUMO: -0.89798 factor:1 | -1 (0.21535) | -1 | -1 |
| G: -5683.64846 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.00299 HOMO: -6.63141 LUMO: -0.91430 factor:1 | 1 (-0.98883) | -1 | -1 |
| G: -5683.64846 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.04908 HOMO: -6.63414 LUMO: 0.04354 factor:1 | 1 (-1.03493) | -1 | -1 |
| G: -5683.64846 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.72238 HOMO: -6.65046 LUMO: -0.73743 factor:1 | 1 (-0.70823) | -1 | -1 |
| G: -5683.64846 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.32865 HOMO: -6.73754 LUMO: -0.71838 factor:1 | 1 (-1.31450) | -1 | -1 |
| G: -5683.64846 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.20563 HOMO: -6.65863 LUMO: -0.60137 factor:1 | 1 (-1.19148) | -1 | -1 |
| G: -5683.64846 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.70698 HOMO: -6.61509 LUMO: -0.47892 factor:1 | 1 (-0.69283) | -1 | -1 |
| G: -5683.64846 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.80962 HOMO: -6.82189 LUMO: -0.64763 factor:1 | 1 (-0.79547) | -1 | -1 |
| G: -5683.64846 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.53353 HOMO: -6.56883 LUMO: -0.51974 factor:1 | 1 (-1.51937) | -1 | -1 |
| G: -5683.64846 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.70809 HOMO: -6.97428 LUMO: -0.95512 factor:1 | 1 (-1.69394) | -1 | -1 |
| G: -5683.64846 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.61342 HOMO: -6.70489 LUMO: -0.04082 factor:1 | 1 (-1.59927) | -1 | -1 |
| G: -5683.64846 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.74557 HOMO: -6.74026 LUMO: 0.02177 factor:1 | 1 (-0.73141) | -1 | -1 |
| G: -5683.64846 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.56232 HOMO: -6.50080 LUMO: -0.89525 factor:1 | 1 (-1.54816) | -1 | -1 |
| G: -5683.64846 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.93207 HOMO: -6.46815 LUMO: -0.61226 factor:1 | 1 (-0.91792) | -1 | -1 |
| G: -5683.64846 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.77553 HOMO: -6.57971 LUMO: -0.64219 factor:1 | 1 (-0.76137) | -1 | -1 |
| G: -5683.64846 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.37361 HOMO: -7.17836 LUMO: 0.37280 factor:1 | 1 (-1.35945) | 1 | 1 |
| G: -5683.64846 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.64729 HOMO: -6.67223 LUMO: 0.12245 factor:1 | 1 (-2.63314) | -1 | -1 |
| G: -5683.64846 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.77877 HOMO: -6.55250 LUMO: 0.22858 factor:1 | 1 (-2.76462) | -1 | -1 |
| G: -5683.64846 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.24573 HOMO: -6.97156 LUMO: -1.12927 factor:1 | 1 (-2.23158) | -1 | -1 |
| G: -5683.64846 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.26300 HOMO: -6.78924 LUMO: -0.84900 factor:1 | 1 (-0.24885) | -1 | -1 |
| G: -5683.64846 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.32938 HOMO: -6.65046 LUMO: -0.65307 factor:1 | 1 (-2.31523) | -1 | -1 |
| G: -5683.64846 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.20089 HOMO: -7.41782 LUMO: 0.08980 factor:1 | 1 (-2.18673) | 1 | 1 |
| G: -5683.64846 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.95428 HOMO: -6.56339 LUMO: -0.68573 factor:1 | 1 (-0.94013) | -1 | -1 |
| G: -5683.64846 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.81574 HOMO: -6.31032 LUMO: -0.31837 factor:1 | 1 (-1.80158) | -1 | -1 |
| G: -5683.64846 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.38854 HOMO: -6.72938 LUMO: -0.45987 factor:1 | 1 (-2.37438) | -1 | -1 |
| G: -5683.64846 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.07147 HOMO: -6.59876 LUMO: -1.03131 factor:1 | 1 (-2.05732) | -1 | -1 |
| G: -5683.64846 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.09566 HOMO: -7.29265 LUMO: 0.29660 factor:1 | 1 (-2.08151) | 1 | 1 |
| G: -5683.64846 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.19775 HOMO: -6.42189 LUMO: -0.51157 factor:1 | 1 (-0.18360) | -1 | -1 |
| G: -5683.64846 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.12890 HOMO: -6.27767 LUMO: -0.52790 factor:1 | 1 (-0.11475) | -1 | -1 |
| G: -5683.64846 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.53892 HOMO: -6.41644 LUMO: -0.44627 factor:1 | 1 (-0.52477) | -1 | -1 |
| G: -5683.64846 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.74698 HOMO: -6.23413 LUMO: -0.52790 factor:1 | 1 (-0.73283) | -1 | -1 |
| G: -5683.64846 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.27243 HOMO: -6.63414 LUMO: -0.44082 factor:1 | 1 (-1.25828) | -1 | -1 |
| G: -5683.64846 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.49222 HOMO: -7.03142 LUMO: 0.47076 factor:1 | 1 (-1.47807) | -1 | -1 |
| G: -5683.64846 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.14508 HOMO: -6.62053 LUMO: -0.14422 factor:1 | 1 (-2.13092) | -1 | -1 |
| G: -5683.64846 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.98162 HOMO: -6.22324 LUMO: 1.96194 factor:1 | 1 (-1.96746) | -1 | -1 |
| G: -5683.64846 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.34230 HOMO: -6.17971 LUMO: 1.71704 factor:1 | 1 (-2.32815) | -1 | -1 |
| G: -5683.64846 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.11299 HOMO: -6.70761 LUMO: 1.68711 factor:1 | 1 (-2.09884) | -1 | -1 |
| G: -5683.64846 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.85661 HOMO: -6.52801 LUMO: 1.56193 factor:1 | 1 (-1.84246) | -1 | -1 |
| G: -5683.64846 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.07672 HOMO: -6.55794 LUMO: 1.52384 factor:1 | 1 (-2.06257) | -1 | -1 |
| G: -5683.64846 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.90036 HOMO: -6.47359 LUMO: 1.82316 factor:1 | 1 (-1.88621) | -1 | -1 |
| G: -5683.64846 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.84459 HOMO: -6.65863 LUMO: 1.83133 factor:1 | 1 (-0.83044) | -1 | -1 |
| G: -5683.64846 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.08978 HOMO: -6.46270 LUMO: 1.90208 factor:1 | 1 (-2.07563) | -1 | -1 |
| G: -5683.64846 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.99019 HOMO: -6.41917 LUMO: 2.03269 factor:1 | 1 (-1.97604) | -1 | -1 |
| G: -5683.64846 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.24736 HOMO: -6.48992 LUMO: 1.87486 factor:1 | 1 (-2.23321) | -1 | -1 |
| G: -5683.64846 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.23569 HOMO: -6.51985 LUMO: 1.69527 factor:1 | 1 (-2.22154) | -1 | -1 |
| G: -5683.64846 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.76758 HOMO: -6.36202 LUMO: 2.05718 factor:1 | 1 (-0.75343) | -1 | -1 |
| G: -5683.64846 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.77285 HOMO: -5.96474 LUMO: 1.88575 factor:1 | 1 (-1.75870) | -1 | -1 |
| G: -5683.64846 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.94782 HOMO: -6.56339 LUMO: 2.04630 factor:1 | 1 (-1.93367) | -1 | -1 |
| G: -5683.64846 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.09621 HOMO: -6.43277 LUMO: 1.98371 factor:1 | 1 (-1.08206) | -1 | -1 |
| G: -5683.64846 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.91365 HOMO: -6.53345 LUMO: 2.06262 factor:1 | 1 (-0.89950) | -1 | -1 |
| G: -5683.64846 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.71607 HOMO: -5.81779 LUMO: 2.11432 factor:1 | 1 (-0.70192) | -1 | -1 |
| G: -5683.64846 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.90217 HOMO: -5.91848 LUMO: 1.86942 factor:1 | 1 (-0.88802) | -1 | -1 |
| G: -5683.64846 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.76716 HOMO: -6.48447 LUMO: 1.70343 factor:1 | 1 (-1.75301) | -1 | -1 |
| G: -5683.64846 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.53327 HOMO: -6.29671 LUMO: -0.89525 factor:1 | 1 (-2.51912) | -1 | -1 |
| G: -5683.64846 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.17542 HOMO: -6.63414 LUMO: -0.76192 factor:1 | 1 (-2.16126) | -1 | -1 |
| G: -5683.64846 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.16546 HOMO: -6.56883 LUMO: -0.86260 factor:1 | 1 (-2.15130) | -1 | -1 |
| G: -5683.64846 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.79259 HOMO: -6.93074 LUMO: -0.27483 factor:1 | 1 (-0.77844) | -1 | -1 |
| G: -5683.64846 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.81243 HOMO: -6.85999 LUMO: -0.01905 factor:1 | 1 (-0.79827) | -1 | -1 |
| G: -5683.64846 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.54689 HOMO: -6.26406 LUMO: 0.21769 factor:1 | 1 (-1.53274) | -1 | -1 |
| G: -5683.64846 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.68259 HOMO: -6.62325 LUMO: 0.31293 factor:1 | 1 (-1.66844) | -1 | -1 |
| G: -5683.64846 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.52243 HOMO: -6.59604 LUMO: 0.19592 factor:1 | 1 (-0.50828) | -1 | -1 |
| G: -5683.64846 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.42001 HOMO: -6.43277 LUMO: -0.27756 factor:1 | 1 (-0.40586) | -1 | -1 |
| G: -5683.64846 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.40991 HOMO: -6.54978 LUMO: -0.46531 factor:1 | 1 (-1.39575) | -1 | -1 |
| G: -5683.64846 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.55870 HOMO: -6.65046 LUMO: -0.15783 factor:1 | 1 (-1.54455) | -1 | -1 |
| G: -5683.64846 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.91288 HOMO: -7.28721 LUMO: 0.23946 factor:1 | 1 (-1.89873) | 1 | 1 |
| G: -5683.64846 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.45788 HOMO: -6.71849 LUMO: -0.56600 factor:1 | 1 (-1.44373) | -1 | -1 |
| G: -5683.64846 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.09947 HOMO: -6.85183 LUMO: -0.84355 factor:1 | 1 (-2.08532) | -1 | -1 |
| G: -5683.64846 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.29981 HOMO: -6.53345 LUMO: -0.84627 factor:1 | 1 (-1.28566) | -1 | -1 |
| G: -5683.64846 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.58962 HOMO: -6.60148 LUMO: -0.63130 factor:1 | 1 (-0.57547) | -1 | -1 |
| G: -5683.64846 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.78613 HOMO: -6.36202 LUMO: -0.60137 factor:1 | 1 (-1.77198) | -1 | -1 |
| G: -5683.64846 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.01721 HOMO: -6.28855 LUMO: -0.52790 factor:1 | 1 (-2.00306) | -1 | -1 |
| G: -5683.64846 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.73230 HOMO: -7.07224 LUMO: 0.41906 factor:1 | 1 (-2.71815) | 1 | 1 |
| G: -5683.64846 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.67126 HOMO: -6.36202 LUMO: -0.24218 factor:1 | 1 (-2.65711) | -1 | -1 |
| G: -5683.64846 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.89389 HOMO: -6.43549 LUMO: 0.14150 factor:1 | 1 (-1.87974) | -1 | -1 |
| G: -5683.64846 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.57549 HOMO: -6.76747 LUMO: -0.40545 factor:1 | 1 (-1.56133) | -1 | -1 |
| G: -5683.64846 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.40908 HOMO: -6.15249 LUMO: -0.51157 factor:1 | 1 (-2.39493) | -1 | -1 |
| G: -5683.64846 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.60047 HOMO: -6.33753 LUMO: -0.02993 factor:1 | 1 (-1.58631) | -1 | -1 |
| G: -5683.64846 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.69394 HOMO: -6.49808 LUMO: -0.83811 factor:1 | 1 (-1.67979) | -1 | -1 |
| G: -5683.64846 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.97341 HOMO: -6.64502 LUMO: -0.46259 factor:1 | 1 (-0.95926) | -1 | -1 |
| G: -5683.64846 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.48928 HOMO: -6.34570 LUMO: 0.22041 factor:1 | 1 (-1.47513) | -1 | -1 |
| G: -5683.64846 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.76184 HOMO: -6.63414 LUMO: -0.13606 factor:1 | 1 (-0.74769) | -1 | -1 |
| G: -5683.64846 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.74094 HOMO: -6.59604 LUMO: -0.79729 factor:1 | 1 (-0.72679) | -1 | -1 |
| G: -5683.64846 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.99681 HOMO: -7.09401 LUMO: 0.31837 factor:1 | 1 (-0.98266) | 1 | 1 |
| G: -5683.64846 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.87791 HOMO: -6.48719 LUMO: -0.31021 factor:1 | 1 (-1.86376) | -1 | -1 |
| G: -5683.64846 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.12394 HOMO: -7.11306 LUMO: 0.39729 factor:1 | 1 (-1.10979) | 1 | 1 |
| G: -5683.64846 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11951.00076 HOMO: -6.95251 LUMO: 0.41089 factor:1 | 1 (-2.98661) | -1 | -1 |
| G: -5683.64846 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.62005 HOMO: -6.61509 LUMO: -0.41906 factor:1 | 1 (-2.60590) | -1 | -1 |
| G: -5683.64846 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.90662 HOMO: -6.25318 LUMO: -0.47348 factor:1 | 1 (-1.89247) | -1 | -1 |
| G: -5683.64846 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.62897 HOMO: -6.77019 LUMO: -0.10340 factor:1 | 1 (-0.61481) | -1 | -1 |
| G: -5683.64846 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.80224 HOMO: -6.54706 LUMO: -0.46259 factor:1 | 1 (-1.78809) | -1 | -1 |
| G: -5683.64846 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.88211 HOMO: -6.34297 LUMO: -0.50341 factor:1 | 1 (-0.86796) | -1 | -1 |
| G: -5683.64846 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.14810 HOMO: -6.20692 LUMO: -0.51974 factor:1 | 1 (-1.13395) | -1 | -1 |
| G: -5683.64846 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.32980 HOMO: -7.03686 LUMO: 0.46804 factor:1 | 1 (-1.31564) | -1 | -1 |
| G: -5683.64846 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.38460 HOMO: -6.47087 LUMO: 0.22585 factor:1 | 1 (-1.37045) | -1 | -1 |
| G: -5683.64846 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.87175 HOMO: -6.41917 LUMO: 0.19320 factor:1 | 1 (-0.85759) | -1 | -1 |
| G: -5683.64846 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.85354 HOMO: -6.61237 LUMO: -0.04354 factor:1 | 1 (-0.83939) | -1 | -1 |
| G: -5683.64846 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.00201 HOMO: -6.56339 LUMO: 0.36735 factor:1 | 1 (-0.98785) | -1 | -1 |
| G: -5683.64846 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.12457 HOMO: -6.54978 LUMO: 1.12655 factor:1 | 1 (-1.11042) | -1 | -1 |
| G: -5683.64846 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.15031 HOMO: -6.43277 LUMO: 1.17553 factor:1 | 1 (-1.13616) | -1 | -1 |
| G: -5683.64846 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.77277 HOMO: -6.29944 LUMO: 1.40955 factor:1 | 1 (-1.75862) | -1 | -1 |
| G: -5683.64846 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.91493 HOMO: -6.74842 LUMO: 0.74015 factor:1 | 1 (-0.90078) | -1 | -1 |
| G: -5683.64846 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.70626 HOMO: -6.15522 LUMO: 1.94289 factor:1 | 1 (-1.69211) | -1 | -1 |
| G: -5683.64846 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.42056 HOMO: -6.20147 LUMO: 1.40139 factor:1 | 1 (-2.40641) | -1 | -1 |
| G: -5683.64846 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.57458 HOMO: -6.41100 LUMO: 1.40139 factor:1 | 1 (-2.56043) | -1 | -1 |
| G: -5683.64846 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.97492 HOMO: -6.74570 LUMO: 1.80956 factor:1 | 1 (-1.96077) | -1 | -1 |
| G: -5683.64846 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.29825 HOMO: -6.60148 LUMO: -1.04764 factor:1 | 1 (-2.28410) | -1 | -1 |
| G: -5683.64846 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.21387 HOMO: -6.82734 LUMO: -0.83267 factor:1 | 1 (-2.19971) | -1 | -1 |
| G: -5683.64846 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.02311 HOMO: -7.01782 LUMO: -0.32382 factor:1 | 1 (-2.00896) | -1 | -1 |
| G: -5683.64846 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.26522 HOMO: -6.54434 LUMO: 0.11157 factor:1 | 1 (-1.25107) | -1 | -1 |
| G: -5683.64846 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.78544 HOMO: -6.53617 LUMO: 0.32926 factor:1 | 1 (-2.77129) | -1 | -1 |
| G: -5683.64846 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11951.66361 HOMO: -6.62597 LUMO: -0.60137 factor:1 | 1 (-3.64946) | -1 | -1 |
| G: -5683.64846 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.77807 HOMO: -6.60965 LUMO: -0.75376 factor:1 | 1 (-2.76391) | -1 | -1 |
| G: -5683.64846 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.95714 HOMO: -6.29399 LUMO: 0.06803 factor:1 | 1 (-2.94299) | -1 | -1 |
| G: -5683.64846 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.17879 HOMO: -6.60692 LUMO: -0.47076 factor:1 | 1 (-2.16464) | -1 | -1 |
| G: -5683.64846 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.13256 HOMO: -7.33891 LUMO: 0.39184 factor:1 | 1 (-2.11841) | 1 | 1 |
| G: -5683.64846 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.80403 HOMO: -6.60692 LUMO: 1.46125 factor:1 | 1 (-2.78987) | -1 | -1 |
| G: -5683.64846 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.22538 HOMO: -6.21780 LUMO: 2.09256 factor:1 | 1 (-2.21122) | -1 | -1 |
| G: -5683.64846 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.40998 HOMO: -6.28311 LUMO: 1.80411 factor:1 | 1 (-2.39583) | -1 | -1 |
| G: -5683.64846 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.99351 HOMO: -6.51168 LUMO: 1.84765 factor:1 | 1 (-1.97936) | -1 | -1 |
| G: -5683.64846 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.18510 HOMO: -6.66951 LUMO: 2.01636 factor:1 | 1 (-2.17095) | -1 | -1 |
| G: -5683.64846 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.01941 HOMO: -6.75387 LUMO: 1.73881 factor:1 | 1 (-2.00526) | -1 | -1 |
| G: -5683.64846 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.93020 HOMO: -6.77291 LUMO: 1.89935 factor:1 | 1 (-0.91604) | -1 | -1 |
| G: -5683.64846 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.17705 HOMO: -6.36474 LUMO: 1.61091 factor:1 | 1 (-2.16290) | -1 | -1 |
| G: -5683.64846 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.48782 HOMO: -6.60420 LUMO: 1.40955 factor:1 | 1 (-0.47367) | -1 | -1 |
| G: -5683.64846 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.23329 HOMO: -6.81645 LUMO: 1.59731 factor:1 | 1 (-2.21914) | -1 | -1 |
| G: -5683.64846 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.28480 HOMO: -5.90215 LUMO: 2.12249 factor:1 | 1 (-0.27064) | -1 | -1 |
| G: -5683.64846 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.33022 HOMO: -6.26950 LUMO: 1.62996 factor:1 | 1 (-2.31607) | -1 | -1 |
| G: -5683.64846 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.22459 HOMO: -6.41100 LUMO: 1.80684 factor:1 | 1 (-2.21044) | -1 | -1 |
| G: -5683.64846 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.93123 HOMO: -6.64230 LUMO: 2.23405 factor:1 | 1 (-0.91708) | -1 | -1 |
| G: -5683.64846 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.36969 HOMO: -6.66951 LUMO: 2.21501 factor:1 | 1 (-1.35554) | -1 | -1 |
| G: -5683.64846 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.42060 HOMO: -6.90897 LUMO: 2.00004 factor:1 | 1 (-1.40645) | -1 | -1 |
| G: -5683.64846 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.56800 HOMO: -6.61781 LUMO: 1.42043 factor:1 | 1 (-1.55385) | -1 | -1 |
| G: -5683.64846 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.67299 HOMO: -6.56611 LUMO: 1.60003 factor:1 | 1 (-1.65883) | -1 | -1 |
| G: -5683.64846 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.52036 HOMO: -6.70489 LUMO: 1.78779 factor:1 | 1 (-1.50620) | -1 | -1 |
| G: -5683.64846 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.52974 HOMO: -6.46815 LUMO: 1.59459 factor:1 | 1 (-1.51559) | -1 | -1 |
| G: -5683.64846 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.69326 HOMO: -6.31304 LUMO: 1.36873 factor:1 | 1 (-1.67911) | -1 | -1 |
| G: -5683.64846 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.70020 HOMO: -6.22597 LUMO: 1.54833 factor:1 | 1 (-1.68604) | -1 | -1 |
| G: -5683.64846 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.58719 HOMO: -5.63004 LUMO: 1.96466 factor:1 | 1 (-1.57304) | -1 | -1 |
| G: -5683.64846 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.98651 HOMO: -7.02598 LUMO: 1.79323 factor:1 | 1 (-1.97236) | -1 | -1 |
| G: -5683.64846 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.81024 HOMO: -6.78924 LUMO: 2.10888 factor:1 | 1 (-1.79609) | -1 | -1 |
| G: -5683.64846 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.06401 HOMO: -6.13345 LUMO: 2.07351 factor:1 | 1 (-2.04986) | -1 | -1 |
| G: -5683.64846 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.31901 HOMO: -6.46270 LUMO: -0.37552 factor:1 | 1 (-2.30486) | -1 | -1 |
| G: -5683.64846 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.03794 HOMO: -6.51985 LUMO: -0.49525 factor:1 | 1 (-2.02379) | -1 | -1 |
| G: -5683.64846 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.43322 HOMO: -6.60965 LUMO: 1.90480 factor:1 | 1 (-2.41907) | -1 | -1 |
| G: -5683.64846 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.51785 HOMO: -6.51168 LUMO: 1.92112 factor:1 | 1 (-1.50370) | -1 | -1 |
| G: -5683.64846 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.65633 HOMO: -6.71305 LUMO: 1.91024 factor:1 | 1 (-1.64218) | -1 | -1 |
| G: -5683.64846 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.78480 HOMO: -6.86815 LUMO: 2.02997 factor:1 | 1 (-1.77064) | -1 | -1 |
| G: -5683.64846 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.99334 HOMO: -6.69944 LUMO: 1.95106 factor:1 | 1 (-1.97919) | -1 | -1 |
| G: -5683.64846 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.77941 HOMO: -6.45182 LUMO: 1.66806 factor:1 | 1 (-1.76526) | -1 | -1 |
| G: -5683.64846 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11951.00177 HOMO: -6.44638 LUMO: 2.16058 factor:1 | 1 (-2.98762) | -1 | -1 |
| G: -5683.64846 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.81253 HOMO: -6.65591 LUMO: 1.95106 factor:1 | 1 (-0.79838) | -1 | -1 |
| G: -5683.64846 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.70701 HOMO: -6.35114 LUMO: 1.42316 factor:1 | 1 (-0.69286) | -1 | -1 |
| G: -5683.64846 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.69864 HOMO: -6.48719 LUMO: 1.59187 factor:1 | 1 (-2.68448) | -1 | -1 |
| G: -5683.64846 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.06418 HOMO: -7.05591 LUMO: 1.61908 factor:1 | 1 (-2.05002) | -1 | -1 |
| G: -5683.64846 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.70836 HOMO: -6.92258 LUMO: 1.87214 factor:1 | 1 (-1.69421) | -1 | -1 |
| G: -5683.64846 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.69323 HOMO: -5.85861 LUMO: 2.11705 factor:1 | 1 (-1.67908) | -1 | -1 |
| G: -5683.64846 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.53826 HOMO: -6.27767 LUMO: 1.75513 factor:1 | 1 (-1.52411) | -1 | -1 |
| G: -5683.64846 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.28808 HOMO: -6.16882 LUMO: 1.73881 factor:1 | 1 (-1.27393) | -1 | -1 |
| G: -5683.64846 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.28560 HOMO: -6.62053 LUMO: 1.39594 factor:1 | 1 (-1.27145) | -1 | -1 |
| G: -5683.64846 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.68526 HOMO: -5.46405 LUMO: 1.68166 factor:1 | 1 (-1.67111) | -1 | -1 |
| G: -5683.64846 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.42117 HOMO: -6.39740 LUMO: 1.68711 factor:1 | 1 (-1.40702) | -1 | -1 |
| G: -5683.64846 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.46889 HOMO: -6.99333 LUMO: 2.08439 factor:1 | 1 (-2.45474) | -1 | -1 |
| G: -5683.64846 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.01313 HOMO: -6.16882 LUMO: 1.71976 factor:1 | 1 (-1.99898) | -1 | -1 |
| G: -5683.64846 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.98009 HOMO: -7.19741 LUMO: 2.24766 factor:1 | 1 (-1.96594) | 1 | 1 |
| G: -5683.64846 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.13825 HOMO: -6.77291 LUMO: 2.17691 factor:1 | 1 (-2.12409) | -1 | -1 |
| G: -5683.64846 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.93343 HOMO: -6.29944 LUMO: 2.16603 factor:1 | 1 (-0.91928) | -1 | -1 |
| G: -5683.64846 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.99950 HOMO: -6.10079 LUMO: 1.83949 factor:1 | 1 (-0.98535) | -1 | -1 |
| G: -5683.64846 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.17064 HOMO: -6.63686 LUMO: 2.05990 factor:1 | 1 (-1.15648) | -1 | -1 |
| G: -5683.64846 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.90840 HOMO: -6.91713 LUMO: 1.87486 factor:1 | 1 (-0.89425) | -1 | -1 |
| G: -5683.64846 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.65073 HOMO: -6.63958 LUMO: 1.79323 factor:1 | 1 (-0.63658) | -1 | -1 |
| G: -5683.64846 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11946.05074 HOMO: -6.61781 LUMO: 1.70071 factor:1 | -1 (1.96341) | -1 | -1 |
| G: -5683.64846 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11946.23597 HOMO: -6.20420 LUMO: 1.82861 factor:1 | -1 (1.77818) | -1 | -1 |
| G: -5683.64846 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.62181 HOMO: -6.47903 LUMO: -2.16875 factor:1 | 1 (-0.60766) | -1 | -1 |
| G: -5683.64846 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.21053 HOMO: -6.53073 LUMO: 2.18235 factor:1 | 1 (-1.19638) | -1 | -1 |
| G: -5683.64846 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.76151 HOMO: -7.01782 LUMO: 1.72520 factor:1 | 1 (-0.74736) | -1 | -1 |
| G: -5683.64846 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.31951 HOMO: -6.66135 LUMO: -0.75648 factor:1 | 1 (-1.30536) | -1 | -1 |
| G: -5683.64846 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.26763 HOMO: -7.56749 LUMO: 0.22585 factor:1 | 1 (-0.25347) | 1 | 1 |
| G: -5683.64846 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.98825 HOMO: -6.45182 LUMO: -0.71294 factor:1 | -1 (0.02591) | -1 | -1 |
| G: -5683.64846 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.39846 HOMO: -6.31032 LUMO: -0.34286 factor:1 | 1 (-0.38431) | -1 | -1 |
| G: -5683.64846 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.00558 HOMO: -6.41917 LUMO: 2.04085 factor:1 | -1 (0.00857) | -1 | -1 |
| G: -5683.64846 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11946.94219 HOMO: -6.61781 LUMO: 1.98915 factor:1 | -1 (1.07197) | -1 | -1 |
| G: -5683.64846 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11946.84869 HOMO: -5.86405 LUMO: 1.57282 factor:1 | -1 (1.16546) | -1 | -1 |
| G: -5683.64846 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.95439 HOMO: -6.44094 LUMO: 1.80956 factor:1 | 1 (-0.94024) | -1 | -1 |
| G: -5683.64846 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.07736 HOMO: -6.59060 LUMO: 2.08167 factor:1 | 1 (-1.06320) | -1 | -1 |
| G: -5683.64846 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.09853 HOMO: -6.20147 LUMO: 1.69799 factor:1 | 1 (-1.08437) | -1 | -1 |
| G: -5683.64846 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.07722 HOMO: -6.50352 LUMO: -0.41361 factor:1 | 1 (-1.06307) | -1 | -1 |
| G: -5683.64846 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.42975 HOMO: -6.10896 LUMO: -0.55783 factor:1 | 1 (-0.41560) | -1 | -1 |
| G: -5683.64846 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.08770 HOMO: -6.74842 LUMO: -0.56872 factor:1 | 1 (-1.07354) | -1 | -1 |
| G: -5683.64846 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.43405 HOMO: -6.59060 LUMO: -0.22041 factor:1 | 1 (-0.41990) | -1 | -1 |
| G: -5683.64846 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.29837 HOMO: -6.22052 LUMO: -0.60137 factor:1 | 1 (-0.28422) | -1 | -1 |
| G: -5683.64846 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.87958 HOMO: -6.65863 LUMO: 0.07891 factor:1 | 1 (-0.86543) | -1 | -1 |
| G: -5683.64846 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.18100 HOMO: -6.57427 LUMO: 1.71160 factor:1 | 1 (-1.16685) | -1 | -1 |
| G: -5683.64846 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.55887 HOMO: -5.84773 LUMO: 1.99459 factor:1 | 1 (-0.54472) | -1 | -1 |
| G: -5683.64846 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.27179 HOMO: -6.02188 LUMO: 1.91296 factor:1 | 1 (-0.25764) | -1 | -1 |
| G: -5683.64846 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.45321 HOMO: -6.17698 LUMO: 2.00004 factor:1 | 1 (-0.43906) | -1 | -1 |
| G: -5683.64846 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.90913 HOMO: -6.02732 LUMO: 1.90752 factor:1 | 1 (-0.89498) | -1 | -1 |
| G: -5683.64846 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.02492 HOMO: -6.68584 LUMO: -0.50885 factor:1 | 1 (-1.01077) | -1 | -1 |
| G: -5683.64846 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.22210 HOMO: -6.61781 LUMO: -0.73471 factor:1 | 1 (-0.20795) | -1 | -1 |
| G: -5683.64846 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.22430 HOMO: -6.66407 LUMO: -0.79729 factor:1 | 1 (-1.21014) | -1 | -1 |
| G: -5683.64846 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.73851 HOMO: -6.56339 LUMO: 0.23130 factor:1 | 1 (-1.72436) | -1 | -1 |
| G: -5683.64846 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.65966 HOMO: -6.76747 LUMO: 0.08980 factor:1 | 1 (-0.64551) | -1 | -1 |
| G: -5683.64846 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.44572 HOMO: -6.70489 LUMO: -0.53334 factor:1 | 1 (-0.43157) | -1 | -1 |
| G: -5683.64846 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.57999 HOMO: -7.28993 LUMO: 0.10885 factor:1 | 1 (-0.56583) | 1 | 1 |
| G: -5683.64846 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.84380 HOMO: -6.22052 LUMO: 0.51974 factor:1 | 1 (-0.82965) | -1 | -1 |
| G: -5683.64846 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.79166 HOMO: -6.81645 LUMO: 0.25307 factor:1 | 1 (-0.77751) | -1 | -1 |
| G: -5683.64846 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.89384 HOMO: -6.80285 LUMO: 0.02721 factor:1 | 1 (-0.87969) | -1 | -1 |
| G: -5683.64846 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.78524 HOMO: -6.51441 LUMO: 0.08163 factor:1 | 1 (-0.77109) | -1 | -1 |
| G: -5683.64846 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.75645 HOMO: -6.73482 LUMO: -0.77008 factor:1 | 1 (-0.74230) | -1 | -1 |
| G: -5683.64846 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.68444 HOMO: -6.29127 LUMO: -0.44355 factor:1 | 1 (-1.67029) | -1 | -1 |
| G: -5683.64846 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.97161 HOMO: -6.72938 LUMO: -0.64763 factor:1 | 1 (-0.95746) | -1 | -1 |
| G: -5683.64846 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.05961 HOMO: -6.49264 LUMO: -0.74559 factor:1 | 1 (-1.04546) | -1 | -1 |
| G: -5683.64846 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11945.71773 HOMO: -6.67223 LUMO: -0.55239 factor:1 | -1 (2.29642) | -1 | -1 |
| G: -5683.64846 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.44011 HOMO: -6.33481 LUMO: 0.33198 factor:1 | 1 (-1.42596) | -1 | -1 |
| G: -5683.64846 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.01246 HOMO: -6.76475 LUMO: -0.25307 factor:1 | 1 (-0.99830) | -1 | -1 |
| G: -5683.64846 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.15322 HOMO: -6.65318 LUMO: 0.03810 factor:1 | 1 (-1.13907) | -1 | -1 |
| G: -5683.64846 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.41552 HOMO: -6.09263 LUMO: 0.21497 factor:1 | 1 (-0.40137) | -1 | -1 |
| G: -5683.64846 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.87054 HOMO: -6.32120 LUMO: -0.85444 factor:1 | 1 (-1.85639) | -1 | -1 |
| G: -5683.64846 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.73195 HOMO: -6.57155 LUMO: -0.67484 factor:1 | 1 (-1.71780) | -1 | -1 |
| G: -5683.64846 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.13259 HOMO: -6.53345 LUMO: -0.78913 factor:1 | 1 (-1.11844) | -1 | -1 |
| G: -5683.64846 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.85166 HOMO: -7.07768 LUMO: 0.28844 factor:1 | 1 (-1.83750) | 1 | 1 |
| G: -5683.64846 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.24566 HOMO: -6.75114 LUMO: 0.18776 factor:1 | 1 (-1.23151) | -1 | -1 |
| G: -5683.64846 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.82850 HOMO: -6.77019 LUMO: -0.12245 factor:1 | 1 (-1.81435) | -1 | -1 |
| G: -5683.64846 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.36574 HOMO: -6.43549 LUMO: 0.16327 factor:1 | 1 (-1.35159) | -1 | -1 |
| G: -5683.64846 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.65584 HOMO: -6.69400 LUMO: -0.16327 factor:1 | 1 (-1.64169) | -1 | -1 |
| G: -5683.64846 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11946.02206 HOMO: -6.38651 LUMO: -0.61770 factor:1 | -1 (1.99209) | -1 | -1 |
| G: -5683.64846 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11946.86363 HOMO: -6.34297 LUMO: -0.33198 factor:1 | -1 (1.15052) | -1 | -1 |
| G: -5683.64846 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.29585 HOMO: -7.51578 LUMO: 0.02177 factor:1 | -1 (0.71830) | 1 | 1 |
| G: -5683.64846 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.45945 HOMO: -6.47359 LUMO: -0.22585 factor:1 | -1 (0.55470) | -1 | -1 |
| G: -5683.64846 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.72817 HOMO: -6.68040 LUMO: -0.47076 factor:1 | 1 (-1.71402) | -1 | -1 |
| G: -5683.64846 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.80485 HOMO: -6.75659 LUMO: -0.57688 factor:1 | 1 (-1.79070) | -1 | -1 |
| G: -5683.64846 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.89685 HOMO: -6.73754 LUMO: -0.61226 factor:1 | 1 (-1.88270) | -1 | -1 |
| G: -5683.64846 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.29181 HOMO: -7.37429 LUMO: 0.31293 factor:1 | 1 (-1.27766) | 1 | 1 |
| G: -5683.64846 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.59658 HOMO: -6.23413 LUMO: -0.90886 factor:1 | 1 (-1.58242) | -1 | -1 |
| G: -5683.64846 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.86926 HOMO: -6.51985 LUMO: -0.68028 factor:1 | 1 (-1.85511) | -1 | -1 |
| G: -5683.64846 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.26677 HOMO: -6.52257 LUMO: -0.77280 factor:1 | 1 (-1.25262) | -1 | -1 |
| G: -5683.64846 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.74938 HOMO: -7.29537 LUMO: 0.31837 factor:1 | 1 (-0.73522) | 1 | 1 |
| G: -5683.64846 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.82549 HOMO: -6.08447 LUMO: 0.25851 factor:1 | 1 (-0.81133) | -1 | -1 |
| G: -5683.64846 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.01319 HOMO: -6.20964 LUMO: 0.13606 factor:1 | 1 (-0.99904) | -1 | -1 |
| G: -5683.64846 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.55732 HOMO: -6.49808 LUMO: -0.14150 factor:1 | 1 (-0.54317) | -1 | -1 |
| G: -5683.64846 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.63359 HOMO: -7.10761 LUMO: 0.28028 factor:1 | 1 (-0.61944) | 1 | 1 |
| G: -5683.64846 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.69637 HOMO: -6.60965 LUMO: -0.62858 factor:1 | 1 (-0.68222) | -1 | -1 |
| G: -5683.64846 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.87632 HOMO: -6.40012 LUMO: -0.26939 factor:1 | 1 (-0.86217) | -1 | -1 |
| G: -5683.64846 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.02293 HOMO: -6.65318 LUMO: -0.73199 factor:1 | 1 (-1.00878) | -1 | -1 |
| G: -5683.64846 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.84326 HOMO: -6.51441 LUMO: -0.44899 factor:1 | 1 (-0.82910) | -1 | -1 |
| G: -5683.64846 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.47353 HOMO: -6.28583 LUMO: -0.48708 factor:1 | 1 (-1.45937) | -1 | -1 |
| G: -5683.64846 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.34043 HOMO: -6.96884 LUMO: 0.19864 factor:1 | 1 (-1.32628) | -1 | -1 |
| G: -5683.64846 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.03357 HOMO: -6.89809 LUMO: 0.34558 factor:1 | 1 (-1.01942) | -1 | -1 |
| G: -5683.64846 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.72045 HOMO: -6.67495 LUMO: -0.15510 factor:1 | 1 (-0.70630) | -1 | -1 |
| G: -5683.64846 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.83988 HOMO: -7.34980 LUMO: 0.19864 factor:1 | 1 (-0.82573) | 1 | 1 |
| G: -5683.64846 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.29444 HOMO: -6.71305 LUMO: -0.81634 factor:1 | -1 (0.71971) | -1 | -1 |
| G: -5683.64846 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.87884 HOMO: -6.39468 LUMO: -0.47076 factor:1 | 1 (-1.86469) | -1 | -1 |
| G: -5683.64846 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.72235 HOMO: -6.31304 LUMO: 1.39594 factor:1 | 1 (-1.70819) | -1 | -1 |
| G: -5683.64846 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.64229 HOMO: -6.57155 LUMO: 1.55105 factor:1 | 1 (-1.62814) | -1 | -1 |
| G: -5683.64846 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.53438 HOMO: -6.68312 LUMO: 1.69255 factor:1 | 1 (-0.52023) | -1 | -1 |
| G: -5683.64846 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.19955 HOMO: -6.61509 LUMO: 1.73881 factor:1 | 1 (-2.18540) | -1 | -1 |
| G: -5683.64846 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.90621 HOMO: -6.17971 LUMO: 1.90208 factor:1 | 1 (-1.89206) | -1 | -1 |
| G: -5683.64846 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.86232 HOMO: -6.53073 LUMO: 1.73337 factor:1 | 1 (-1.84817) | -1 | -1 |
| G: -5683.64846 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.82812 HOMO: -5.91303 LUMO: 1.90480 factor:1 | 1 (-1.81397) | -1 | -1 |
| G: -5683.64846 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.55607 HOMO: -6.42733 LUMO: 1.80139 factor:1 | 1 (-0.54191) | -1 | -1 |
| G: -5683.64846 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.23104 HOMO: -6.78924 LUMO: 2.31569 factor:1 | 1 (-2.21688) | -1 | -1 |
| G: -5683.64846 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.46590 HOMO: -6.04093 LUMO: 1.91568 factor:1 | 1 (-2.45175) | -1 | -1 |
| G: -5683.64846 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.50339 HOMO: -6.90081 LUMO: 2.36739 factor:1 | 1 (-2.48924) | -1 | -1 |
| G: -5683.64846 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.97517 HOMO: -6.60965 LUMO: 2.18507 factor:1 | 1 (-1.96102) | -1 | -1 |
| G: -5683.64846 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.19367 HOMO: -6.75387 LUMO: 2.48712 factor:1 | 1 (-2.17952) | -1 | -1 |
| G: -5683.64846 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.80538 HOMO: -6.56883 LUMO: 1.71432 factor:1 | 1 (-0.79123) | -1 | -1 |
| G: -5683.64846 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.66814 HOMO: -6.41644 LUMO: 1.72792 factor:1 | 1 (-1.65399) | -1 | -1 |
| G: -5683.64846 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.47456 HOMO: -6.92530 LUMO: 2.54426 factor:1 | 1 (-1.46041) | -1 | -1 |
| G: -5683.64846 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.08682 HOMO: -6.41644 LUMO: 2.70209 factor:1 | 1 (-1.07267) | -1 | -1 |
| G: -5683.64846 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.88500 HOMO: -6.29671 LUMO: 2.14698 factor:1 | 1 (-0.87085) | -1 | -1 |
| G: -5683.64846 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.63473 HOMO: -6.29127 LUMO: 1.87486 factor:1 | 1 (-1.62057) | -1 | -1 |
| G: -5683.64846 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.42970 HOMO: -6.75931 LUMO: 2.78917 factor:1 | 1 (-0.41555) | -1 | -1 |
| G: -5683.64846 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.17727 HOMO: -6.40828 LUMO: 1.86942 factor:1 | 1 (-2.16311) | -1 | -1 |
| G: -5683.64846 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.65097 HOMO: -6.45726 LUMO: 1.97010 factor:1 | 1 (-1.63682) | -1 | -1 |
| G: -5683.64846 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.00094 HOMO: -6.43277 LUMO: 1.22723 factor:1 | 1 (-1.98678) | -1 | -1 |
| G: -5683.64846 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.30772 HOMO: -6.63414 LUMO: 1.62452 factor:1 | 1 (-2.29357) | -1 | -1 |
| G: -5683.64846 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.54551 HOMO: -6.54162 LUMO: 2.16058 factor:1 | 1 (-0.53136) | -1 | -1 |
| G: -5683.64846 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.60187 HOMO: -6.40284 LUMO: 1.88575 factor:1 | 1 (-2.58772) | -1 | -1 |
| G: -5683.64846 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.90001 HOMO: -6.20964 LUMO: 1.84221 factor:1 | 1 (-1.88586) | -1 | -1 |
| G: -5683.64846 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.75122 HOMO: -6.58516 LUMO: 1.69799 factor:1 | 1 (-1.73707) | -1 | -1 |
| G: -5683.64846 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.80265 HOMO: -6.44094 LUMO: 2.05446 factor:1 | 1 (-1.78850) | -1 | -1 |
| G: -5683.64846 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.53784 HOMO: -6.61509 LUMO: 2.16058 factor:1 | 1 (-2.52369) | -1 | -1 |
| G: -5683.64846 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.37295 HOMO: -6.65591 LUMO: 1.69527 factor:1 | 1 (-1.35880) | -1 | -1 |
| G: -5683.64846 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.97805 HOMO: -5.55112 LUMO: 1.80411 factor:1 | 1 (-1.96390) | -1 | -1 |
| G: -5683.64846 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.98964 HOMO: -6.68312 LUMO: 2.38100 factor:1 | 1 (-1.97549) | -1 | -1 |
| G: -5683.64846 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.20408 HOMO: -6.51168 LUMO: 2.14698 factor:1 | 1 (-1.18993) | -1 | -1 |
| G: -5683.64846 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.23262 HOMO: -6.04637 LUMO: 1.48302 factor:1 | 1 (-1.21847) | -1 | -1 |
| G: -5683.64846 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.51927 HOMO: -6.81645 LUMO: -0.74287 factor:1 | 1 (-1.50512) | -1 | -1 |
| G: -5683.64846 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.48536 HOMO: -6.96884 LUMO: -0.97961 factor:1 | 1 (-1.47121) | -1 | -1 |
| G: -5683.64846 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.30046 HOMO: -6.45998 LUMO: 0.09796 factor:1 | 1 (-1.28631) | -1 | -1 |
| G: -5683.64846 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.61209 HOMO: -6.44638 LUMO: 0.09524 factor:1 | 1 (-1.59793) | -1 | -1 |
| G: -5683.64846 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.47040 HOMO: -6.16338 LUMO: -0.54151 factor:1 | 1 (-1.45624) | -1 | -1 |
| G: -5683.64846 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.47587 HOMO: -6.35930 LUMO: -0.47892 factor:1 | 1 (-1.46171) | -1 | -1 |
| G: -5683.64846 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.82651 HOMO: -6.65318 LUMO: -0.00272 factor:1 | 1 (-1.81236) | -1 | -1 |
| G: -5683.64846 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.38969 HOMO: -6.50080 LUMO: 0.14694 factor:1 | 1 (-1.37554) | -1 | -1 |
| G: -5683.64846 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.49581 HOMO: -6.60420 LUMO: 0.94968 factor:1 | 1 (-1.48166) | -1 | -1 |
| G: -5683.64846 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.41829 HOMO: -6.60148 LUMO: -0.77552 factor:1 | 1 (-1.40413) | -1 | -1 |
| G: -5683.64846 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.42765 HOMO: -6.81645 LUMO: -1.05580 factor:1 | 1 (-1.41350) | -1 | -1 |
| G: -5683.64846 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.52836 HOMO: -6.57971 LUMO: -0.82178 factor:1 | 1 (-1.51420) | -1 | -1 |
| G: -5683.64846 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.67693 HOMO: -6.09263 LUMO: -0.45171 factor:1 | 1 (-1.66278) | -1 | -1 |
| G: -5683.64846 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.52457 HOMO: -6.74298 LUMO: -0.61770 factor:1 | 1 (-1.51042) | -1 | -1 |
| G: -5683.64846 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.51334 HOMO: -6.72393 LUMO: 1.21091 factor:1 | 1 (-1.49918) | -1 | -1 |
| G: -5683.64846 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.42786 HOMO: -6.30488 LUMO: 1.70071 factor:1 | 1 (-1.41371) | -1 | -1 |
| G: -5683.64846 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.99258 HOMO: -6.38107 LUMO: 1.55649 factor:1 | 1 (-1.97843) | -1 | -1 |
| G: -5683.64846 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.13093 HOMO: -6.17154 LUMO: 1.46669 factor:1 | 1 (-1.11678) | -1 | -1 |
| G: -5683.64846 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.39293 HOMO: -6.86543 LUMO: 1.98643 factor:1 | 1 (-1.37877) | -1 | -1 |
| G: -5683.64846 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.29785 HOMO: -6.69944 LUMO: 1.65173 factor:1 | 1 (-1.28370) | -1 | -1 |
| G: -5683.64846 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.53527 HOMO: -6.77836 LUMO: 2.16331 factor:1 | 1 (-1.52112) | -1 | -1 |
| G: -5683.64846 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.42465 HOMO: -6.42189 LUMO: 2.36467 factor:1 | 1 (-1.41050) | -1 | -1 |
| G: -5683.64846 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.55181 HOMO: -7.00965 LUMO: 2.04358 factor:1 | 1 (-1.53766) | -1 | -1 |
| G: -5683.64846 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.45701 HOMO: -6.36746 LUMO: 2.13881 factor:1 | 1 (-1.44286) | -1 | -1 |
| G: -5683.64846 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.63297 HOMO: -6.37835 LUMO: 1.89935 factor:1 | 1 (-0.61881) | -1 | -1 |
| G: -5683.64846 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.44479 HOMO: -7.03959 LUMO: 1.27349 factor:1 | 1 (-1.43064) | -1 | -1 |
| G: -5683.64846 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.79594 HOMO: -6.67495 LUMO: -0.89253 factor:1 | 1 (-2.78179) | -1 | -1 |
| G: -5683.64846 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.35761 HOMO: -6.71849 LUMO: -0.97961 factor:1 | 1 (-1.34345) | -1 | -1 |
| G: -5683.64846 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.20886 HOMO: -6.47903 LUMO: 0.01633 factor:1 | 1 (-2.19471) | -1 | -1 |
| G: -5683.64846 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.79442 HOMO: -6.38379 LUMO: 0.01088 factor:1 | 1 (-2.78027) | -1 | -1 |
| G: -5683.64846 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.29636 HOMO: -6.49536 LUMO: -0.55239 factor:1 | 1 (-0.28221) | -1 | -1 |
| G: -5683.64846 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.25907 HOMO: -6.53345 LUMO: -0.53879 factor:1 | 1 (-1.24492) | -1 | -1 |
| G: -5683.64846 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.94239 HOMO: -6.16610 LUMO: 2.15514 factor:1 | 1 (-0.92823) | -1 | -1 |
| G: -5683.64846 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.04314 HOMO: -6.35114 LUMO: 1.98643 factor:1 | 1 (-2.02899) | -1 | -1 |
| G: -5683.64846 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.43167 HOMO: -6.43277 LUMO: 2.16058 factor:1 | 1 (-1.41752) | -1 | -1 |
| G: -5683.64846 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.22289 HOMO: -6.89809 LUMO: 2.20684 factor:1 | 1 (-0.20874) | -1 | -1 |
| G: -5683.64846 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.12361 HOMO: -6.54434 LUMO: 1.93473 factor:1 | 1 (-1.10946) | -1 | -1 |
| G: -5683.64846 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.22313 HOMO: -6.72938 LUMO: 2.03269 factor:1 | 1 (-1.20897) | -1 | -1 |
| G: -5683.64846 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.16332 HOMO: -6.90353 LUMO: 2.19868 factor:1 | 1 (-0.14917) | -1 | -1 |
| G: -5683.64846 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.16311 HOMO: -6.41372 LUMO: 2.02453 factor:1 | 1 (-0.14896) | -1 | -1 |
| G: -5683.64846 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.22357 HOMO: -6.46543 LUMO: 1.90752 factor:1 | 1 (-0.20942) | -1 | -1 |
| G: -5683.64846 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.22548 HOMO: -6.55522 LUMO: 2.11977 factor:1 | 1 (-0.21132) | -1 | -1 |
| G: -5683.64846 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.21157 HOMO: -6.28855 LUMO: 2.02181 factor:1 | 1 (-0.19742) | -1 | -1 |
| G: -5683.64846 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.27655 HOMO: -6.45726 LUMO: 1.52112 factor:1 | 1 (-0.26240) | -1 | -1 |
| G: -5683.64846 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.99992 HOMO: -6.37291 LUMO: 2.11705 factor:1 | -1 (0.01423) | -1 | -1 |
| G: -5683.64846 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.05116 HOMO: -6.88448 LUMO: 2.24494 factor:1 | 1 (-0.03701) | -1 | -1 |
| G: -5683.64846 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.80973 HOMO: -6.86271 LUMO: 2.41637 factor:1 | 1 (-0.79558) | -1 | -1 |
| G: -5683.64846 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.16901 HOMO: -6.69400 LUMO: 2.34562 factor:1 | 1 (-0.15486) | -1 | -1 |
| G: -5683.64846 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.34714 HOMO: -6.18243 LUMO: 2.53882 factor:1 | 1 (-0.33299) | -1 | -1 |
| G: -5683.64846 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.98316 HOMO: -6.61237 LUMO: 2.54154 factor:1 | -1 (0.03099) | -1 | -1 |
| G: -5683.64846 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.35054 HOMO: -6.69672 LUMO: 2.16331 factor:1 | 1 (-0.33639) | -1 | -1 |
| G: -5683.64846 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.75966 HOMO: -6.33481 LUMO: 2.34018 factor:1 | 1 (-0.74551) | -1 | -1 |
| G: -5683.64846 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.43623 HOMO: -5.99739 LUMO: 2.37283 factor:1 | 1 (-0.42208) | -1 | -1 |
| G: -5683.64846 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.85678 HOMO: -6.49808 LUMO: 2.47351 factor:1 | 1 (-0.84263) | -1 | -1 |
| G: -5683.64846 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.85956 HOMO: -6.22052 LUMO: 1.86398 factor:1 | 1 (-0.84540) | -1 | -1 |
| G: -5683.64846 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.44156 HOMO: -6.32665 LUMO: 2.28031 factor:1 | 1 (-0.42741) | -1 | -1 |
| G: -5683.64846 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.25742 HOMO: -5.98378 LUMO: 2.16331 factor:1 | 1 (-0.24327) | -1 | -1 |
| G: -5683.64846 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.49219 HOMO: -6.08991 LUMO: 2.30208 factor:1 | 1 (-1.47804) | -1 | -1 |
| G: -5683.64846 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.55432 HOMO: -7.07224 LUMO: 1.55105 factor:1 | 1 (-1.54016) | 1 | 1 |
| G: -5683.64846 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.21782 HOMO: -6.84638 LUMO: 1.76874 factor:1 | 1 (-1.20367) | -1 | -1 |
| G: -5683.64846 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.95066 HOMO: -6.68856 LUMO: 1.47758 factor:1 | 1 (-0.93651) | -1 | -1 |
| G: -5683.64846 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.98130 HOMO: -6.69672 LUMO: 1.71976 factor:1 | 1 (-0.96715) | -1 | -1 |
| G: -5683.64846 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.99074 HOMO: -6.86543 LUMO: 2.24766 factor:1 | 1 (-0.97659) | -1 | -1 |
| G: -5683.64846 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.06630 HOMO: -7.21646 LUMO: 1.71976 factor:1 | 1 (-2.05215) | 1 | 1 |
| G: -5683.64846 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.91253 HOMO: -6.94162 LUMO: 2.21773 factor:1 | 1 (-1.89838) | -1 | -1 |
| G: -5683.64846 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.91860 HOMO: -6.34842 LUMO: 2.04358 factor:1 | 1 (-1.90444) | -1 | -1 |
| G: -5683.64846 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.29314 HOMO: -6.53345 LUMO: 1.96738 factor:1 | 1 (-1.27899) | -1 | -1 |
| G: -5683.64846 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.74474 HOMO: -6.34842 LUMO: 1.88303 factor:1 | 1 (-1.73059) | -1 | -1 |
| G: -5683.64846 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.76213 HOMO: -6.38651 LUMO: 2.08983 factor:1 | 1 (-1.74798) | -1 | -1 |
| G: -5683.64846 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.20808 HOMO: -6.01372 LUMO: 1.43676 factor:1 | 1 (-1.19393) | -1 | -1 |
| G: -5683.64846 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.29277 HOMO: -6.30216 LUMO: 1.41771 factor:1 | 1 (-0.27862) | -1 | -1 |
| G: -5683.64846 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.32863 HOMO: -6.52801 LUMO: 1.77146 factor:1 | 1 (-0.31448) | -1 | -1 |
| G: -5683.64846 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.23089 HOMO: -6.53617 LUMO: 1.72792 factor:1 | 1 (-0.21674) | -1 | -1 |
| G: -5683.64846 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.09350 HOMO: -6.56611 LUMO: 2.20412 factor:1 | 1 (-0.07935) | -1 | -1 |
| G: -5683.64846 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.50569 HOMO: -6.66679 LUMO: -0.72927 factor:1 | 1 (-1.49154) | -1 | -1 |
| G: -5683.64846 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.11707 HOMO: -6.85455 LUMO: -0.85444 factor:1 | 1 (-0.10291) | -1 | -1 |
| G: -5683.64846 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.11088 HOMO: -7.21646 LUMO: 0.27211 factor:1 | 1 (-1.09673) | 1 | 1 |
| G: -5683.64846 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.00745 HOMO: -6.57971 LUMO: -0.41361 factor:1 | 1 (-0.99330) | -1 | -1 |
| G: -5683.64846 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.93188 HOMO: -7.03142 LUMO: -1.14288 factor:1 | 1 (-0.91773) | -1 | -1 |
| G: -5683.64846 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.85825 HOMO: -6.29944 LUMO: 0.06803 factor:1 | 1 (-0.84410) | -1 | -1 |
| G: -5683.64846 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.86287 HOMO: -6.47359 LUMO: 0.28028 factor:1 | 1 (-0.84872) | -1 | -1 |
| G: -5683.64846 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.02824 HOMO: -6.42189 LUMO: 1.61364 factor:1 | 1 (-1.01409) | -1 | -1 |
| G: -5683.64846 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.03956 HOMO: -6.41100 LUMO: 1.80956 factor:1 | 1 (-1.02541) | -1 | -1 |
| G: -5683.64846 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.63000 HOMO: -6.83278 LUMO: 1.83949 factor:1 | 1 (-0.61585) | -1 | -1 |
| G: -5683.64846 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.70649 HOMO: -6.78380 LUMO: -0.76192 factor:1 | 1 (-0.69234) | -1 | -1 |
| G: -5683.64846 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.43587 HOMO: -6.95795 LUMO: 2.13609 factor:1 | 1 (-0.42172) | -1 | -1 |
| G: -5683.64846 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.69787 HOMO: -6.57155 LUMO: 1.89119 factor:1 | 1 (-0.68371) | -1 | -1 |
| G: -5683.64846 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.84726 HOMO: -6.65591 LUMO: 1.93745 factor:1 | 1 (-0.83310) | -1 | -1 |
| G: -5683.64846 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.25687 HOMO: -6.44638 LUMO: 2.26943 factor:1 | 1 (-1.24272) | -1 | -1 |
| G: -5683.64846 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.00216 HOMO: -5.88038 LUMO: 1.90480 factor:1 | 1 (-1.98801) | -1 | -1 |
| G: -5683.64846 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.60944 HOMO: -6.22052 LUMO: 2.17691 factor:1 | 1 (-2.59529) | -1 | -1 |
| G: -5683.64846 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.83098 HOMO: -6.04637 LUMO: 2.23950 factor:1 | 1 (-0.81683) | -1 | -1 |
| G: -5683.64846 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.87898 HOMO: -6.44366 LUMO: 2.24766 factor:1 | 1 (-0.86483) | -1 | -1 |
| G: -5683.64846 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.84352 HOMO: -6.81917 LUMO: 2.08439 factor:1 | 1 (-1.82937) | -1 | -1 |
| G: -5683.64846 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.73104 HOMO: -6.48447 LUMO: 2.28576 factor:1 | 1 (-0.71688) | -1 | -1 |
| G: -5683.64846 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.71770 HOMO: -6.54434 LUMO: 1.99187 factor:1 | 1 (-0.70355) | -1 | -1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.75027 HOMO: -6.17698 LUMO: -0.65852 factor:1 | 1 (-1.73611) | -1 | -1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.11303 HOMO: -6.08174 LUMO: -0.58504 factor:1 | 1 (-1.09888) | -1 | -1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.69911 HOMO: -6.55250 LUMO: -0.86804 factor:1 | 1 (-1.68496) | -1 | -1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.69991 HOMO: -6.57699 LUMO: -0.89525 factor:1 | 1 (-0.68575) | -1 | -1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.32383 HOMO: -6.63141 LUMO: -1.04220 factor:1 | -1 (0.69033) | -1 | -1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11946.74733 HOMO: -6.69128 LUMO: -0.76736 factor:1 | -1 (1.26683) | -1 | -1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.29313 HOMO: -6.25318 LUMO: -1.03131 factor:1 | -1 (0.72102) | -1 | -1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.06424 HOMO: -6.69944 LUMO: 0.01905 factor:1 | 1 (-1.05009) | -1 | -1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.65952 HOMO: -6.28583 LUMO: 0.38368 factor:1 | 1 (-0.64537) | -1 | -1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.55526 HOMO: -6.90081 LUMO: -0.83811 factor:1 | -1 (0.45889) | -1 | -1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.96446 HOMO: -6.78380 LUMO: -0.10068 factor:1 | 1 (-0.95030) | -1 | -1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.00378 HOMO: -6.30488 LUMO: -0.98505 factor:1 | 1 (-0.98962) | -1 | -1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.66334 HOMO: -6.29671 LUMO: -1.79051 factor:1 | -1 (0.35081) | -1 | -1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.78908 HOMO: -6.76747 LUMO: -0.22041 factor:1 | 1 (-0.77493) | -1 | -1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.17115 HOMO: -6.22597 LUMO: -0.94968 factor:1 | 1 (-1.15700) | -1 | -1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.23390 HOMO: -6.73482 LUMO: 0.05987 factor:1 | 1 (-1.21975) | -1 | -1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.35067 HOMO: -6.28855 LUMO: 0.34831 factor:1 | 1 (-1.33651) | -1 | -1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.38822 HOMO: -6.69400 LUMO: 0.25307 factor:1 | 1 (-1.37407) | -1 | -1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11946.96899 HOMO: -6.70216 LUMO: 0.61226 factor:1 | -1 (1.04516) | -1 | -1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.87806 HOMO: -6.70216 LUMO: 0.17415 factor:1 | 1 (-0.86391) | -1 | -1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.01165 HOMO: -6.70761 LUMO: 0.24762 factor:1 | -1 (0.00250) | -1 | -1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.80824 HOMO: -6.68856 LUMO: -0.84900 factor:1 | -1 (0.20591) | -1 | -1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.02858 HOMO: -6.71033 LUMO: -0.38640 factor:1 | -1 (0.98557) | -1 | -1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.12437 HOMO: -6.24501 LUMO: -0.09252 factor:1 | -1 (0.88979) | -1 | -1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.08945 HOMO: -6.81645 LUMO: -0.07347 factor:1 | -1 (0.92470) | -1 | -1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.12148 HOMO: -6.49536 LUMO: 0.09796 factor:1 | -1 (0.89267) | -1 | -1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.06628 HOMO: -6.71033 LUMO: -0.26395 factor:1 | 1 (-1.05213) | -1 | -1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.23421 HOMO: -6.70489 LUMO: -0.09252 factor:1 | 1 (-0.22006) | -1 | -1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.57833 HOMO: -6.23685 LUMO: 0.39729 factor:1 | 1 (-0.56417) | -1 | -1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.11796 HOMO: -6.69400 LUMO: -0.05442 factor:1 | 1 (-0.10381) | -1 | -1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.03003 HOMO: -6.36202 LUMO: 0.09796 factor:1 | 1 (-1.01588) | -1 | -1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.72003 HOMO: -6.54978 LUMO: 0.15510 factor:1 | 1 (-1.70588) | -1 | -1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.21200 HOMO: -6.77836 LUMO: 0.25851 factor:1 | 1 (-1.19785) | -1 | -1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.15099 HOMO: -5.70623 LUMO: 0.73471 factor:1 | 1 (-1.13684) | -1 | -1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.68130 HOMO: -5.58378 LUMO: 0.89253 factor:1 | -1 (0.33285) | -1 | -1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.80448 HOMO: -5.68718 LUMO: 0.87893 factor:1 | 1 (-0.79033) | -1 | -1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.95290 HOMO: -5.10486 LUMO: 1.11567 factor:1 | -1 (0.06125) | -1 | -1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.82928 HOMO: -4.59328 LUMO: 1.27621 factor:1 | -1 (0.18487) | -1 | -1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.12704 HOMO: -4.45450 LUMO: 1.82044 factor:1 | 1 (-1.11289) | -1 | -1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.30122 HOMO: -4.64226 LUMO: 1.70615 factor:1 | 1 (-1.28707) | -1 | -1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.49312 HOMO: -5.04227 LUMO: 1.04492 factor:1 | 1 (-1.47897) | -1 | -1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.21710 HOMO: -4.85723 LUMO: 0.93607 factor:1 | 1 (-2.20295) | -1 | -1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.56858 HOMO: -4.72934 LUMO: 1.00410 factor:1 | 1 (-1.55442) | -1 | -1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.93552 HOMO: -4.56335 LUMO: 1.56738 factor:1 | 1 (-1.92137) | -1 | -1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.99948 HOMO: -5.48854 LUMO: 0.33198 factor:1 | 1 (-0.98532) | -1 | -1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.45899 HOMO: -4.97424 LUMO: 1.33608 factor:1 | 1 (-2.44483) | -1 | -1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.76233 HOMO: -4.60145 LUMO: 1.74697 factor:1 | 1 (-0.74818) | -1 | -1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.31064 HOMO: -5.60010 LUMO: 0.74831 factor:1 | 1 (-1.29649) | -1 | -1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.12182 HOMO: -5.66541 LUMO: 0.66668 factor:1 | 1 (-1.10767) | -1 | -1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.02687 HOMO: -6.50080 LUMO: 0.07075 factor:1 | 1 (-2.01272) | -1 | -1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.08233 HOMO: -5.79603 LUMO: 0.22313 factor:1 | 1 (-2.06817) | -1 | -1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.66752 HOMO: -4.68036 LUMO: 1.29798 factor:1 | 1 (-0.65337) | -1 | -1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.13983 HOMO: -4.84363 LUMO: 1.34424 factor:1 | 1 (-1.12568) | -1 | -1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.63785 HOMO: -4.62321 LUMO: 1.82861 factor:1 | 1 (-2.62369) | -1 | -1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.82388 HOMO: -5.83684 LUMO: 0.82178 factor:1 | 1 (-0.80973) | -1 | -1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.06881 HOMO: -5.27629 LUMO: 0.57960 factor:1 | 1 (-1.05466) | -1 | -1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.28340 HOMO: -5.15928 LUMO: -2.96876 factor:1 | 1 (-1.26925) | -1 | -1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.17993 HOMO: -5.08853 LUMO: 0.89253 factor:1 | 1 (-2.16578) | -1 | -1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.02346 HOMO: -6.42461 LUMO: 0.04354 factor:1 | 1 (-0.00931) | -1 | -1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.83799 HOMO: -6.42733 LUMO: -0.00544 factor:1 | -1 (0.17617) | -1 | -1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.64160 HOMO: -5.87494 LUMO: 0.69933 factor:1 | -1 (0.37255) | -1 | -1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11946.74635 HOMO: -5.07492 LUMO: 1.02587 factor:1 | -1 (1.26781) | -1 | -1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.79651 HOMO: -4.44362 LUMO: 1.99187 factor:1 | 1 (-0.78235) | -1 | -1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.63996 HOMO: -5.82052 LUMO: 0.43810 factor:1 | 1 (-0.62581) | -1 | -1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.97888 HOMO: -5.75793 LUMO: 0.76464 factor:1 | 1 (-0.96473) | -1 | -1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.63999 HOMO: -5.09669 LUMO: 0.72382 factor:1 | 1 (-0.62583) | -1 | -1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.71196 HOMO: -6.75387 LUMO: -2.02453 factor:1 | 1 (-0.69781) | -1 | -1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.61735 HOMO: -5.02322 LUMO: 1.14832 factor:1 | 1 (-0.60319) | -1 | -1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.31114 HOMO: -5.75521 LUMO: 0.73471 factor:1 | 1 (-0.29699) | -1 | -1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.09859 HOMO: -5.89943 LUMO: 0.54967 factor:1 | 1 (-0.08444) | -1 | -1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.07990 HOMO: -5.80147 LUMO: 0.72382 factor:1 | 1 (-2.06575) | -1 | -1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.96785 HOMO: -6.16066 LUMO: 0.39457 factor:1 | 1 (-1.95370) | -1 | -1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.30638 HOMO: -5.98650 LUMO: 0.76736 factor:1 | 1 (-2.29223) | -1 | -1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.81740 HOMO: -4.74839 LUMO: 1.88847 factor:1 | 1 (-1.80324) | -1 | -1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.80174 HOMO: -5.62459 LUMO: 0.26939 factor:1 | -1 (0.21241) | -1 | -1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.43047 HOMO: -4.88172 LUMO: 1.30070 factor:1 | -1 (0.58368) | -1 | -1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.03184 HOMO: -5.09397 LUMO: 0.98505 factor:1 | 1 (-0.01769) | -1 | -1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11946.66664 HOMO: -6.50080 LUMO: -0.28300 factor:1 | -1 (1.34751) | -1 | -1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.64898 HOMO: -5.04227 LUMO: 1.49935 factor:1 | -1 (0.36518) | -1 | -1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.55381 HOMO: -5.22731 LUMO: 0.88437 factor:1 | 1 (-0.53966) | -1 | -1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.45655 HOMO: -4.95519 LUMO: 1.25717 factor:1 | 1 (-0.44240) | -1 | -1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.70366 HOMO: -4.61233 LUMO: 1.27621 factor:1 | 1 (-0.68951) | -1 | -1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.90430 HOMO: -4.70757 LUMO: 1.63813 factor:1 | -1 (0.10985) | -1 | -1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.33587 HOMO: -4.85179 LUMO: 1.11839 factor:1 | 1 (-0.32172) | -1 | -1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.65399 HOMO: -4.97696 LUMO: 1.00138 factor:1 | 1 (-1.63984) | -1 | -1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.30018 HOMO: -5.64636 LUMO: 0.81090 factor:1 | 1 (-2.28603) | -1 | -1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.00798 HOMO: -4.37831 LUMO: 1.90208 factor:1 | 1 (-1.99383) | -1 | -1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.26304 HOMO: -4.67764 LUMO: 1.54561 factor:1 | 1 (-2.24888) | -1 | -1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.47059 HOMO: -5.87766 LUMO: 0.42994 factor:1 | 1 (-1.45644) | -1 | -1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.09393 HOMO: -6.03821 LUMO: 0.32382 factor:1 | 1 (-1.07978) | -1 | -1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.43793 HOMO: -5.99739 LUMO: 0.69389 factor:1 | 1 (-1.42378) | -1 | -1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.97084 HOMO: -6.43821 LUMO: 0.15238 factor:1 | 1 (-1.95669) | -1 | -1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.79572 HOMO: -6.63414 LUMO: -0.07347 factor:1 | 1 (-0.78157) | -1 | -1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.40853 HOMO: -6.50080 LUMO: 0.10068 factor:1 | 1 (-0.39437) | -1 | -1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.46445 HOMO: -6.49264 LUMO: 0.19592 factor:1 | 1 (-0.45029) | -1 | -1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.51095 HOMO: -5.83956 LUMO: 0.12517 factor:1 | 1 (-0.49680) | -1 | -1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.50461 HOMO: -6.50896 LUMO: 0.19048 factor:1 | 1 (-0.49046) | -1 | -1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.31682 HOMO: -6.56611 LUMO: 0.04898 factor:1 | 1 (-0.30267) | -1 | -1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.94486 HOMO: -6.68040 LUMO: -0.08436 factor:1 | 1 (-0.93071) | -1 | -1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.93252 HOMO: -6.73754 LUMO: -0.08708 factor:1 | -1 (0.08163) | -1 | -1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.95352 HOMO: -6.80285 LUMO: -0.10612 factor:1 | -1 (0.06063) | -1 | -1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.93513 HOMO: -6.35658 LUMO: 0.02177 factor:1 | -1 (0.07902) | -1 | -1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.58235 HOMO: -5.74160 LUMO: 0.14694 factor:1 | 1 (-0.56820) | -1 | -1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.94513 HOMO: -4.78376 LUMO: 0.92791 factor:1 | 1 (-1.93097) | -1 | -1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.37262 HOMO: -5.90215 LUMO: 0.36463 factor:1 | 1 (-2.35847) | -1 | -1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.99435 HOMO: -4.99329 LUMO: 0.85988 factor:1 | 1 (-1.98020) | -1 | -1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.36113 HOMO: -4.93887 LUMO: 1.33608 factor:1 | 1 (-2.34698) | -1 | -1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.65965 HOMO: -5.19193 LUMO: 0.50341 factor:1 | 1 (-1.64550) | -1 | -1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.86286 HOMO: -6.64502 LUMO: -1.98643 factor:1 | 1 (-2.84871) | -1 | -1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.32663 HOMO: -5.15384 LUMO: 0.94968 factor:1 | 1 (-2.31248) | -1 | -1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.06586 HOMO: -6.31032 LUMO: 0.08436 factor:1 | 1 (-2.05171) | -1 | -1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.00015 HOMO: -4.88716 LUMO: 0.82995 factor:1 | 1 (-1.98600) | -1 | -1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.70822 HOMO: -5.57017 LUMO: 0.19320 factor:1 | 1 (-1.69407) | -1 | -1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.48378 HOMO: -4.92254 LUMO: 0.93879 factor:1 | 1 (-2.46962) | -1 | -1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.78499 HOMO: -4.77288 LUMO: 1.60003 factor:1 | 1 (-1.77084) | -1 | -1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.04711 HOMO: -4.97696 LUMO: 0.89798 factor:1 | 1 (-2.03296) | -1 | -1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.98405 HOMO: -5.00690 LUMO: 1.14288 factor:1 | 1 (-0.96990) | -1 | -1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.92864 HOMO: -4.88444 LUMO: 1.48574 factor:1 | 1 (-0.91449) | -1 | -1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.94132 HOMO: -5.03955 LUMO: 1.51023 factor:1 | 1 (-1.92716) | -1 | -1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.70470 HOMO: -5.22459 LUMO: 0.99049 factor:1 | 1 (-2.69055) | -1 | -1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.93232 HOMO: -5.29534 LUMO: 0.96056 factor:1 | 1 (-0.91817) | -1 | -1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.40542 HOMO: -5.35520 LUMO: 0.68301 factor:1 | 1 (-1.39126) | -1 | -1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.63113 HOMO: -5.27357 LUMO: 1.18642 factor:1 | 1 (-2.61697) | -1 | -1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.35507 HOMO: -5.79875 LUMO: 0.61770 factor:1 | 1 (-1.34092) | -1 | -1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.00432 HOMO: -7.64640 LUMO: -2.45175 factor:1 | 1 (-0.99017) | -1 | -1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.19820 HOMO: -7.46953 LUMO: -1.29798 factor:1 | 1 (-1.18405) | 1 | 1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.66523 HOMO: -7.95389 LUMO: -0.37280 factor:1 | 1 (-1.65108) | 1 | 1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.62270 HOMO: -7.23279 LUMO: -1.19186 factor:1 | 1 (-1.60855) | 1 | 1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.48479 HOMO: -7.14299 LUMO: -1.12927 factor:1 | 1 (-1.47064) | 1 | 1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.71967 HOMO: -6.93074 LUMO: 0.31565 factor:1 | 1 (-2.70552) | -1 | -1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.62937 HOMO: -6.63141 LUMO: 0.28028 factor:1 | 1 (-0.61522) | -1 | -1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.42806 HOMO: -7.10489 LUMO: -1.07213 factor:1 | 1 (-1.41390) | 1 | 1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.62862 HOMO: -7.00693 LUMO: -0.69389 factor:1 | 1 (-2.61447) | -1 | -1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.58687 HOMO: -8.50356 LUMO: -1.79595 factor:1 | 1 (-0.57272) | -1 | -1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.36680 HOMO: -7.79334 LUMO: -2.33746 factor:1 | 1 (-1.35265) | -1 | -1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.95714 HOMO: -7.24367 LUMO: -0.85172 factor:1 | 1 (-0.94298) | 1 | 1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.80823 HOMO: -7.94028 LUMO: -0.20136 factor:1 | 1 (-1.79407) | 1 | 1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.99548 HOMO: -7.22462 LUMO: 0.84627 factor:1 | -1 (0.01867) | 1 | 1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.70725 HOMO: -6.54978 LUMO: 0.34831 factor:1 | 1 (-0.69310) | -1 | -1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.94855 HOMO: -6.86815 LUMO: 0.32109 factor:1 | 1 (-1.93440) | -1 | -1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.55774 HOMO: -7.17564 LUMO: -1.28438 factor:1 | 1 (-1.54359) | 1 | 1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.94651 HOMO: -7.03142 LUMO: -1.12655 factor:1 | 1 (-1.93236) | -1 | -1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.52342 HOMO: -7.39878 LUMO: 0.15783 factor:1 | 1 (-2.50927) | 1 | 1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.92663 HOMO: -7.25728 LUMO: 0.42178 factor:1 | 1 (-0.91248) | 1 | 1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.51726 HOMO: -6.86543 LUMO: 0.93879 factor:1 | 1 (-0.50311) | -1 | -1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.96272 HOMO: -7.09673 LUMO: -0.69661 factor:1 | -1 (0.05143) | 1 | 1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.51152 HOMO: -7.74708 LUMO: 0.01088 factor:1 | 1 (-0.49737) | 1 | 1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.10509 HOMO: -6.80557 LUMO: 0.46531 factor:1 | 1 (-0.09094) | -1 | -1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.44791 HOMO: -7.29265 LUMO: 1.31975 factor:1 | -1 (0.56624) | 1 | 1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.55015 HOMO: -6.93618 LUMO: 0.29388 factor:1 | 1 (-1.53600) | -1 | -1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.80287 HOMO: -6.53073 LUMO: 0.71022 factor:1 | 1 (-1.78871) | -1 | -1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.35843 HOMO: -6.41917 LUMO: -1.24084 factor:1 | 1 (-0.34428) | -1 | -1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.28179 HOMO: -6.67495 LUMO: -1.09118 factor:1 | 1 (-1.26764) | -1 | -1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.77885 HOMO: -6.97156 LUMO: -0.53606 factor:1 | 1 (-0.76469) | -1 | -1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.46423 HOMO: -6.85183 LUMO: -0.45715 factor:1 | 1 (-0.45008) | -1 | -1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.49846 HOMO: -7.12666 LUMO: -0.67484 factor:1 | 1 (-0.48431) | 1 | 1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.81218 HOMO: -7.49946 LUMO: -0.14694 factor:1 | 1 (-0.79803) | 1 | 1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.69738 HOMO: -7.44231 LUMO: 0.58232 factor:1 | 1 (-0.68322) | 1 | 1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.37729 HOMO: -7.36340 LUMO: -0.68301 factor:1 | 1 (-0.36314) | 1 | 1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.35174 HOMO: -6.13073 LUMO: -0.54967 factor:1 | 1 (-0.33758) | -1 | -1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.69792 HOMO: -7.81511 LUMO: -0.06531 factor:1 | 1 (-0.68377) | 1 | 1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.36385 HOMO: -7.26816 LUMO: -1.02587 factor:1 | 1 (-0.34969) | 1 | 1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.28455 HOMO: -7.98110 LUMO: -0.17960 factor:1 | 1 (-0.27040) | 1 | 1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.72627 HOMO: -7.44776 LUMO: -1.00954 factor:1 | 1 (-0.71212) | 1 | 1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.56880 HOMO: -7.47769 LUMO: -1.02859 factor:1 | 1 (-0.55465) | 1 | 1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.38103 HOMO: -6.75659 LUMO: 0.39457 factor:1 | 1 (-1.36688) | -1 | -1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.27507 HOMO: -6.71849 LUMO: 0.36735 factor:1 | 1 (-1.26092) | -1 | -1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.16770 HOMO: -7.64096 LUMO: -1.43948 factor:1 | 1 (-1.15355) | 1 | 1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.02291 HOMO: -7.83144 LUMO: -1.36601 factor:1 | 1 (-1.00875) | 1 | 1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.95558 HOMO: -7.19469 LUMO: 0.35103 factor:1 | 1 (-1.94142) | 1 | 1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.98690 HOMO: -7.03414 LUMO: 0.20409 factor:1 | 1 (-0.97275) | -1 | -1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.06644 HOMO: -7.22734 LUMO: 0.31293 factor:1 | 1 (-1.05229) | 1 | 1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.03251 HOMO: -6.93618 LUMO: 0.56055 factor:1 | 1 (-1.01836) | -1 | -1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.09069 HOMO: -6.94707 LUMO: -0.88709 factor:1 | 1 (-1.07654) | -1 | -1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.94393 HOMO: -6.86543 LUMO: -0.83267 factor:1 | 1 (-1.92978) | -1 | -1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.81931 HOMO: -6.82189 LUMO: -1.15376 factor:1 | 1 (-0.80516) | -1 | -1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.71585 HOMO: -6.65046 LUMO: -0.46531 factor:1 | 1 (-0.70170) | -1 | -1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.63903 HOMO: -6.52529 LUMO: 0.20953 factor:1 | 1 (-1.62487) | -1 | -1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.61707 HOMO: -6.80557 LUMO: 0.44355 factor:1 | 1 (-0.60292) | -1 | -1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.61577 HOMO: -6.93074 LUMO: -0.81634 factor:1 | 1 (-0.60162) | -1 | -1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.31938 HOMO: -7.43143 LUMO: -0.45987 factor:1 | 1 (-0.30523) | 1 | 1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11946.84523 HOMO: -7.07224 LUMO: -0.68028 factor:1 | -1 (1.16892) | 1 | 1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.81210 HOMO: -6.68040 LUMO: -0.71566 factor:1 | 1 (-0.79795) | -1 | -1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.61821 HOMO: -6.26406 LUMO: -1.09934 factor:1 | 1 (-1.60406) | -1 | -1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.76918 HOMO: -5.94569 LUMO: -0.72110 factor:1 | 1 (-1.75503) | -1 | -1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.42082 HOMO: -6.12256 LUMO: -0.42178 factor:1 | 1 (-1.40667) | -1 | -1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.68499 HOMO: -6.09807 LUMO: 0.11429 factor:1 | 1 (-1.67083) | -1 | -1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.70670 HOMO: -7.35252 LUMO: -0.55783 factor:1 | 1 (-1.69255) | 1 | 1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.39859 HOMO: -7.57837 LUMO: -0.76736 factor:1 | 1 (-1.38443) | 1 | 1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.61456 HOMO: -6.16066 LUMO: 0.01905 factor:1 | 1 (-1.60041) | -1 | -1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.56252 HOMO: -6.13345 LUMO: -0.41906 factor:1 | 1 (-0.54836) | -1 | -1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.83948 HOMO: -6.10351 LUMO: -0.33742 factor:1 | -1 (0.17467) | -1 | -1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.11961 HOMO: -7.24639 LUMO: -0.51702 factor:1 | 1 (-2.10545) | 1 | 1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.65560 HOMO: -6.98244 LUMO: -1.82044 factor:1 | 1 (-1.64145) | -1 | -1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.35831 HOMO: -6.37563 LUMO: -1.67622 factor:1 | 1 (-1.34416) | -1 | -1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11946.41418 HOMO: -5.79058 LUMO: -2.55243 factor:1 | -1 (1.59998) | -1 | -1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.23058 HOMO: -6.34025 LUMO: -0.27483 factor:1 | 1 (-1.21643) | -1 | -1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.05627 HOMO: -6.05453 LUMO: -0.51157 factor:1 | 1 (-1.04211) | -1 | -1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.22117 HOMO: -7.53755 LUMO: -0.38912 factor:1 | 1 (-1.20702) | 1 | 1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.84568 HOMO: -7.00421 LUMO: -0.50885 factor:1 | 1 (-0.83153) | -1 | -1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.96914 HOMO: -7.52123 LUMO: -0.37552 factor:1 | 1 (-0.95498) | 1 | 1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.18012 HOMO: -6.70489 LUMO: -1.04764 factor:1 | -1 (0.83403) | -1 | -1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.78085 HOMO: -7.06408 LUMO: -1.16737 factor:1 | 1 (-1.76670) | 1 | 1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.00069 HOMO: -6.71849 LUMO: -1.02315 factor:1 | 1 (-1.98654) | -1 | -1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.67037 HOMO: -6.16610 LUMO: -0.50885 factor:1 | 1 (-1.65622) | -1 | -1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.50977 HOMO: -6.48447 LUMO: 0.07619 factor:1 | 1 (-1.49562) | -1 | -1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.69867 HOMO: -7.06135 LUMO: 0.09796 factor:1 | 1 (-1.68452) | 1 | 1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.36721 HOMO: -6.47359 LUMO: 0.22585 factor:1 | 1 (-1.35306) | -1 | -1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.61702 HOMO: -6.10896 LUMO: -0.62314 factor:1 | 1 (-0.60287) | -1 | -1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.78081 HOMO: -6.88176 LUMO: -0.96600 factor:1 | 1 (-0.76665) | -1 | -1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.39993 HOMO: -6.67495 LUMO: 0.21769 factor:1 | 1 (-0.38578) | -1 | -1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.87877 HOMO: -6.84911 LUMO: 0.38368 factor:1 | 1 (-0.86461) | -1 | -1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.02692 HOMO: -6.83550 LUMO: 1.29798 factor:1 | -1 (0.98723) | -1 | -1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.52532 HOMO: -6.67495 LUMO: 1.46941 factor:1 | 1 (-0.51117) | -1 | -1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.64369 HOMO: -6.81917 LUMO: 1.30887 factor:1 | 1 (-0.62954) | -1 | -1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.33353 HOMO: -6.56611 LUMO: 0.66396 factor:1 | 1 (-0.31938) | -1 | -1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.81974 HOMO: -6.76203 LUMO: 0.60137 factor:1 | 1 (-0.80559) | -1 | -1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11946.93095 HOMO: -6.55794 LUMO: 0.34286 factor:1 | -1 (1.08320) | -1 | -1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.60218 HOMO: -6.83550 LUMO: 0.35919 factor:1 | 1 (-1.58803) | -1 | -1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.87501 HOMO: -7.17836 LUMO: 0.63130 factor:1 | 1 (-0.86086) | 1 | 1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.20221 HOMO: -6.29944 LUMO: -0.69389 factor:1 | 1 (-0.18806) | -1 | -1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.37188 HOMO: -7.06680 LUMO: -0.95784 factor:1 | 1 (-2.35773) | 1 | 1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.70648 HOMO: -6.84638 LUMO: -0.87076 factor:1 | 1 (-1.69233) | -1 | -1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.41671 HOMO: -6.96339 LUMO: -1.05308 factor:1 | 1 (-1.40256) | -1 | -1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.47434 HOMO: -6.75387 LUMO: -1.04220 factor:1 | 1 (-1.46019) | -1 | -1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.50003 HOMO: -6.71849 LUMO: -0.84355 factor:1 | 1 (-1.48588) | -1 | -1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.34261 HOMO: -7.16748 LUMO: 0.51702 factor:1 | 1 (-1.32846) | 1 | 1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.96752 HOMO: -6.92530 LUMO: 0.71566 factor:1 | 1 (-1.95337) | -1 | -1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.94372 HOMO: -7.11034 LUMO: 0.01905 factor:1 | 1 (-0.92957) | 1 | -1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.72818 HOMO: -6.79468 LUMO: 0.77008 factor:1 | 1 (-0.71403) | -1 | -1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.63070 HOMO: -6.52801 LUMO: 0.98233 factor:1 | 1 (-1.61655) | -1 | -1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.10590 HOMO: -6.76475 LUMO: 0.53334 factor:1 | 1 (-1.09175) | -1 | -1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.05205 HOMO: -5.29261 LUMO: 0.57416 factor:1 | 1 (-1.03790) | -1 | -1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.43843 HOMO: -6.57971 LUMO: 0.12789 factor:1 | 1 (-0.42428) | -1 | -1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.58083 HOMO: -6.99333 LUMO: 0.51430 factor:1 | 1 (-0.56668) | -1 | -1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.17347 HOMO: -6.41917 LUMO: 0.19048 factor:1 | 1 (-0.15932) | -1 | -1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.00817 HOMO: -6.16066 LUMO: 1.77146 factor:1 | 1 (-1.99402) | -1 | -1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.98941 HOMO: -6.90353 LUMO: 1.65717 factor:1 | 1 (-0.97526) | -1 | -1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.66356 HOMO: -5.94569 LUMO: 1.29526 factor:1 | 1 (-2.64941) | -1 | -1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.52019 HOMO: -6.60420 LUMO: 1.33880 factor:1 | 1 (-1.50604) | -1 | -1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.94807 HOMO: -6.23957 LUMO: 0.09524 factor:1 | 1 (-0.93392) | -1 | -1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.73984 HOMO: -6.80013 LUMO: 1.34696 factor:1 | 1 (-1.72569) | -1 | -1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.79359 HOMO: -7.53483 LUMO: -1.52384 factor:1 | 1 (-0.77944) | -1 | -1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.09365 HOMO: -7.62463 LUMO: -1.65717 factor:1 | 1 (-1.07950) | -1 | -1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.04897 HOMO: -7.62463 LUMO: -1.61364 factor:1 | 1 (-1.03482) | -1 | -1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.59263 HOMO: -8.04096 LUMO: -1.66806 factor:1 | 1 (-1.57848) | -1 | -1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.27826 HOMO: -7.18381 LUMO: -1.17553 factor:1 | 1 (-1.26410) | 1 | 1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.72862 HOMO: -7.69538 LUMO: -1.36601 factor:1 | -1 (0.28553) | 1 | 1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.54626 HOMO: -7.95117 LUMO: -1.48302 factor:1 | 1 (-1.53211) | -1 | -1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.37380 HOMO: -6.98516 LUMO: 0.35919 factor:1 | 1 (-1.35964) | -1 | -1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.81902 HOMO: -7.91579 LUMO: -0.32109 factor:1 | -1 (0.19513) | 1 | 1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.38877 HOMO: -6.75659 LUMO: -0.03537 factor:1 | 1 (-0.37462) | -1 | -1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.60075 HOMO: -7.78518 LUMO: -2.36467 factor:1 | 1 (-0.58660) | -1 | -1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.41337 HOMO: -7.96477 LUMO: -2.75651 factor:1 | 1 (-0.39922) | -1 | -1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.05940 HOMO: -7.60286 LUMO: -2.35106 factor:1 | 1 (-1.04524) | -1 | -1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.15883 HOMO: -7.38245 LUMO: -1.21635 factor:1 | 1 (-0.14468) | 1 | 1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.30600 HOMO: -7.91579 LUMO: -1.50479 factor:1 | 1 (-2.29185) | -1 | -1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.42242 HOMO: -8.07362 LUMO: -0.28028 factor:1 | 1 (-1.40827) | 1 | 1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.70910 HOMO: -7.38245 LUMO: -1.15921 factor:1 | 1 (-0.69495) | 1 | 1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.91548 HOMO: -7.18653 LUMO: -0.94968 factor:1 | -1 (0.09867) | 1 | 1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.60779 HOMO: -6.88448 LUMO: 0.38096 factor:1 | 1 (-1.59363) | -1 | -1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.79521 HOMO: -6.97972 LUMO: 0.43266 factor:1 | -1 (0.21894) | -1 | -1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.38005 HOMO: -6.88992 LUMO: -0.43538 factor:1 | 1 (-1.36590) | -1 | -1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.43603 HOMO: -7.97021 LUMO: -0.17143 factor:1 | 1 (-1.42188) | 1 | 1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.62972 HOMO: -6.92530 LUMO: 0.77280 factor:1 | 1 (-1.61557) | -1 | -1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.66081 HOMO: -7.89674 LUMO: -0.09796 factor:1 | -1 (0.35334) | 1 | 1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.18431 HOMO: -7.02870 LUMO: 0.88709 factor:1 | 1 (-2.17016) | -1 | -1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.40310 HOMO: -6.78380 LUMO: 0.22041 factor:1 | 1 (-1.38895) | -1 | -1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.35412 HOMO: -7.24911 LUMO: -0.82178 factor:1 | 1 (-1.33997) | 1 | 1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.47394 HOMO: -6.77019 LUMO: 0.52790 factor:1 | 1 (-0.45979) | -1 | -1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.54337 HOMO: -8.56070 LUMO: -1.83405 factor:1 | -1 (0.47078) | -1 | -1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.63470 HOMO: -7.74164 LUMO: -2.36195 factor:1 | 1 (-1.62055) | -1 | -1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.68499 HOMO: -7.39878 LUMO: -2.41637 factor:1 | 1 (-0.67084) | -1 | -1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.82696 HOMO: -7.61647 LUMO: -2.34018 factor:1 | -1 (0.18719) | -1 | -1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.66470 HOMO: -6.93346 LUMO: -0.57688 factor:1 | -1 (0.34945) | -1 | -1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.79974 HOMO: -6.85183 LUMO: -1.00410 factor:1 | 1 (-0.78559) | -1 | -1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.82364 HOMO: -7.18925 LUMO: -1.12655 factor:1 | 1 (-0.80948) | 1 | 1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.52804 HOMO: -6.85183 LUMO: -1.60275 factor:1 | 1 (-0.51389) | -1 | -1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.90935 HOMO: -7.51578 LUMO: 0.12517 factor:1 | 1 (-0.89520) | 1 | 1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.01420 HOMO: -7.36068 LUMO: 0.05714 factor:1 | 1 (-1.00005) | 1 | 1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.97577 HOMO: -7.49674 LUMO: 0.18776 factor:1 | 1 (-0.96162) | 1 | 1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.61201 HOMO: -7.09401 LUMO: -1.24900 factor:1 | 1 (-0.59786) | 1 | 1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11946.82956 HOMO: -7.22462 LUMO: -1.61364 factor:1 | -1 (1.18459) | -1 | -1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11946.92657 HOMO: -7.74436 LUMO: -0.18776 factor:1 | -1 (1.08758) | 1 | 1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11945.77950 HOMO: -7.35252 LUMO: 0.75376 factor:1 | -1 (2.23465) | 1 | 1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11945.68758 HOMO: -7.75252 LUMO: 0.00816 factor:1 | -1 (2.32657) | 1 | 1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11945.90478 HOMO: -7.06680 LUMO: 0.24490 factor:1 | -1 (2.10937) | 1 | 1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.48442 HOMO: -7.49129 LUMO: 0.14150 factor:1 | 1 (-0.47027) | 1 | 1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.09282 HOMO: -6.90625 LUMO: -1.11295 factor:1 | 1 (-0.07867) | -1 | -1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.64216 HOMO: -6.78380 LUMO: -0.93063 factor:1 | 1 (-0.62801) | -1 | -1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.02915 HOMO: -7.79878 LUMO: 0.30477 factor:1 | 1 (-0.01499) | 1 | 1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.74480 HOMO: -7.87498 LUMO: 0.61770 factor:1 | 1 (-0.73065) | 1 | 1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.10787 HOMO: -7.23823 LUMO: 0.30205 factor:1 | 1 (-0.09372) | 1 | 1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.50153 HOMO: -7.67633 LUMO: 0.13061 factor:1 | 1 (-0.48738) | 1 | 1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.84356 HOMO: -7.79606 LUMO: 0.34558 factor:1 | -1 (0.17059) | 1 | 1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.23177 HOMO: -6.66135 LUMO: -2.60141 factor:1 | -1 (0.78238) | -1 | -1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.46260 HOMO: -7.03142 LUMO: 0.50885 factor:1 | -1 (0.55155) | -1 | -1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11946.97206 HOMO: -7.05591 LUMO: -0.06531 factor:1 | -1 (1.04209) | -1 | -1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.24995 HOMO: -7.45592 LUMO: -1.39594 factor:1 | -1 (0.76420) | 1 | 1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.36082 HOMO: -7.22462 LUMO: -1.10478 factor:1 | 1 (-0.34667) | 1 | 1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.03505 HOMO: -8.14709 LUMO: -0.55783 factor:1 | 1 (-0.02090) | 1 | 1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.15522 HOMO: -7.22190 LUMO: -1.14560 factor:1 | 1 (-0.14106) | 1 | 1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.35623 HOMO: -7.28721 LUMO: -1.14016 factor:1 | 1 (-0.34207) | 1 | 1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.07198 HOMO: -6.97156 LUMO: 0.51702 factor:1 | 1 (-0.05782) | -1 | -1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.12482 HOMO: -7.37156 LUMO: 0.29388 factor:1 | 1 (-0.11067) | 1 | -1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.69224 HOMO: -7.66273 LUMO: -1.59731 factor:1 | -1 (0.32191) | -1 | -1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.65131 HOMO: -7.50490 LUMO: -1.49935 factor:1 | 1 (-0.63715) | -1 | -1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.71917 HOMO: -7.61102 LUMO: -1.45581 factor:1 | 1 (-0.70502) | 1 | 1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.43536 HOMO: -7.58653 LUMO: -1.61091 factor:1 | 1 (-0.42121) | -1 | -1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.08262 HOMO: -7.36068 LUMO: -1.14560 factor:1 | 1 (-0.06846) | 1 | 1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.14668 HOMO: -6.96339 LUMO: 0.26939 factor:1 | 1 (-2.13253) | -1 | -1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.68019 HOMO: -6.53617 LUMO: 0.22313 factor:1 | 1 (-2.66604) | -1 | -1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.15563 HOMO: -7.33619 LUMO: -1.02587 factor:1 | 1 (-2.14148) | 1 | 1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.78077 HOMO: -6.87904 LUMO: 0.33742 factor:1 | 1 (-1.76662) | -1 | -1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.26603 HOMO: -6.88448 LUMO: 0.58777 factor:1 | 1 (-2.25188) | -1 | -1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.66069 HOMO: -6.55522 LUMO: -1.51295 factor:1 | 1 (-1.64653) | -1 | -1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.52419 HOMO: -7.43415 LUMO: 0.10612 factor:1 | 1 (-1.51004) | 1 | 1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.92312 HOMO: -7.54300 LUMO: -0.02449 factor:1 | 1 (-0.90897) | 1 | 1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.05921 HOMO: -7.42054 LUMO: 0.28028 factor:1 | 1 (-1.04505) | 1 | 1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.97909 HOMO: -6.98244 LUMO: -0.95784 factor:1 | 1 (-0.96494) | -1 | -1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.79183 HOMO: -6.96884 LUMO: -1.12383 factor:1 | 1 (-0.77767) | -1 | -1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.96130 HOMO: -6.80829 LUMO: -0.98233 factor:1 | 1 (-0.94715) | -1 | -1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.93137 HOMO: -7.60830 LUMO: 0.58504 factor:1 | 1 (-0.91721) | 1 | 1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.49468 HOMO: -7.52123 LUMO: 0.08163 factor:1 | 1 (-0.48053) | 1 | 1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.90753 HOMO: -7.59742 LUMO: 0.00272 factor:1 | 1 (-0.89338) | 1 | 1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.83501 HOMO: -6.99333 LUMO: -1.33880 factor:1 | 1 (-0.82086) | -1 | -1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.97977 HOMO: -6.63958 LUMO: -1.39322 factor:1 | 1 (-1.96561) | -1 | -1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.63245 HOMO: -7.86137 LUMO: 0.01633 factor:1 | 1 (-0.61830) | 1 | 1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.93055 HOMO: -7.29537 LUMO: 0.14694 factor:1 | 1 (-0.91640) | 1 | 1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.78102 HOMO: -6.95523 LUMO: 0.48708 factor:1 | 1 (-0.76687) | -1 | -1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.42450 HOMO: -7.10217 LUMO: -1.10478 factor:1 | 1 (-0.41035) | 1 | 1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.07395 HOMO: -6.88176 LUMO: -0.96328 factor:1 | 1 (-1.05980) | -1 | -1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.11737 HOMO: -7.89130 LUMO: -0.13334 factor:1 | -1 (0.89678) | 1 | 1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11946.75875 HOMO: -7.75252 LUMO: 0.25579 factor:1 | -1 (1.25540) | 1 | 1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11946.70403 HOMO: -6.87632 LUMO: -0.93063 factor:1 | -1 (1.31012) | -1 | -1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11946.42688 HOMO: -6.78108 LUMO: -0.86804 factor:1 | -1 (1.58727) | -1 | -1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.53550 HOMO: -5.98106 LUMO: 0.10340 factor:1 | -1 (0.47865) | -1 | -1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.70372 HOMO: -6.40284 LUMO: -0.87349 factor:1 | -1 (0.31043) | -1 | -1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.95297 HOMO: -6.77019 LUMO: -1.20819 factor:1 | 1 (-0.93882) | -1 | -1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.45114 HOMO: -6.90081 LUMO: -1.00682 factor:1 | 1 (-0.43699) | -1 | -1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.81906 HOMO: -6.59060 LUMO: -0.26667 factor:1 | 1 (-0.80491) | -1 | -1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.41397 HOMO: -6.50896 LUMO: -0.48708 factor:1 | 1 (-0.39982) | -1 | -1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.81487 HOMO: -6.20420 LUMO: -0.73471 factor:1 | 1 (-0.80072) | -1 | -1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.59503 HOMO: -6.17154 LUMO: -0.68573 factor:1 | 1 (-0.58088) | -1 | -1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.46640 HOMO: -6.21236 LUMO: 0.09796 factor:1 | 1 (-1.45224) | -1 | -1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.06554 HOMO: -6.38379 LUMO: 0.58232 factor:1 | 1 (-2.05138) | -1 | -1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.91697 HOMO: -7.42871 LUMO: 0.40273 factor:1 | 1 (-0.90282) | 1 | 1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.66826 HOMO: -6.54978 LUMO: 0.26395 factor:1 | 1 (-0.65411) | -1 | -1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.91281 HOMO: -7.14027 LUMO: 0.14150 factor:1 | 1 (-0.89866) | 1 | 1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.72355 HOMO: -7.25456 LUMO: -0.15783 factor:1 | 1 (-0.70940) | 1 | 1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.53680 HOMO: -6.90897 LUMO: 0.63403 factor:1 | 1 (-0.52265) | -1 | -1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.80935 HOMO: -6.49264 LUMO: 0.71022 factor:1 | 1 (-0.79520) | -1 | -1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.06684 HOMO: -6.56067 LUMO: -1.03947 factor:1 | -1 (0.94731) | -1 | -1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.92347 HOMO: -6.79196 LUMO: -1.12655 factor:1 | 1 (-0.90932) | -1 | -1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.84236 HOMO: -6.95251 LUMO: -1.09118 factor:1 | 1 (-0.82821) | -1 | -1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.67650 HOMO: -7.47225 LUMO: -0.22041 factor:1 | 1 (-0.66235) | 1 | 1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.71163 HOMO: -7.13483 LUMO: -0.98505 factor:1 | 1 (-0.69748) | 1 | 1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.75811 HOMO: -6.99061 LUMO: -1.05852 factor:1 | 1 (-0.74396) | -1 | -1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.66918 HOMO: -6.52257 LUMO: -1.11022 factor:1 | 1 (-0.65503) | -1 | -1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.37302 HOMO: -6.75114 LUMO: -1.09934 factor:1 | 1 (-0.35886) | -1 | -1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.67917 HOMO: -6.82189 LUMO: -0.89253 factor:1 | 1 (-0.66502) | -1 | -1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.00415 HOMO: -6.83278 LUMO: -0.97961 factor:1 | -1 (1.01001) | -1 | -1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.22985 HOMO: -6.65318 LUMO: -0.84355 factor:1 | 1 (-1.21570) | -1 | -1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.96900 HOMO: -6.75931 LUMO: -0.88437 factor:1 | 1 (-0.95485) | -1 | -1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.41741 HOMO: -6.19059 LUMO: -0.45715 factor:1 | -1 (0.59675) | -1 | -1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.40780 HOMO: -7.09673 LUMO: -2.01908 factor:1 | -1 (0.60635) | -1 | -1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.68587 HOMO: -7.88042 LUMO: 0.38640 factor:1 | -1 (0.32828) | 1 | 1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.71695 HOMO: -7.83144 LUMO: 0.14422 factor:1 | -1 (0.29720) | 1 | 1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.65423 HOMO: -7.46408 LUMO: 0.44627 factor:1 | -1 (0.35993) | 1 | 1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.79576 HOMO: -7.12394 LUMO: -2.04902 factor:1 | 1 (-1.78161) | -1 | -1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.38197 HOMO: -6.78380 LUMO: -1.11295 factor:1 | 1 (-0.36782) | -1 | -1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.79811 HOMO: -7.12938 LUMO: -0.23674 factor:1 | 1 (-0.78396) | 1 | 1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.96396 HOMO: -6.14705 LUMO: -0.20409 factor:1 | 1 (-1.94980) | -1 | -1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.27684 HOMO: -6.50080 LUMO: -0.28300 factor:1 | 1 (-1.26269) | -1 | -1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.24601 HOMO: -6.50352 LUMO: -0.62042 factor:1 | 1 (-1.23186) | -1 | -1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.00043 HOMO: -6.46543 LUMO: -0.53879 factor:1 | 1 (-0.98628) | -1 | -1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.70565 HOMO: -7.32803 LUMO: -0.52790 factor:1 | 1 (-0.69150) | 1 | 1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.76962 HOMO: -5.94025 LUMO: -0.17687 factor:1 | 1 (-0.75547) | -1 | -1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.85240 HOMO: -5.62187 LUMO: 0.05714 factor:1 | 1 (-0.83825) | -1 | -1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.71754 HOMO: -7.03414 LUMO: -1.04492 factor:1 | 1 (-0.70339) | -1 | -1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.53237 HOMO: -6.75387 LUMO: -2.02181 factor:1 | 1 (-0.51821) | -1 | -1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.90206 HOMO: -6.55250 LUMO: -0.75648 factor:1 | 1 (-0.88791) | -1 | -1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.03016 HOMO: -6.81101 LUMO: -1.02043 factor:1 | -1 (0.98399) | -1 | -1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.73394 HOMO: -6.69672 LUMO: -2.81910 factor:1 | 1 (-1.71979) | -1 | -1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.40171 HOMO: -6.69128 LUMO: -2.58236 factor:1 | 1 (-1.38756) | -1 | -1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.50830 HOMO: -6.73482 LUMO: -2.06807 factor:1 | 1 (-1.49415) | -1 | -1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.41905 HOMO: -7.66545 LUMO: 0.17143 factor:1 | 1 (-1.40490) | 1 | 1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.07823 HOMO: -6.87904 LUMO: -1.25172 factor:1 | 1 (-1.06407) | -1 | -1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.44221 HOMO: -6.84366 LUMO: -0.19320 factor:1 | 1 (-1.42805) | -1 | -1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.38188 HOMO: -6.97972 LUMO: -0.97961 factor:1 | 1 (-1.36773) | -1 | -1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11945.80459 HOMO: -6.72121 LUMO: -0.70477 factor:1 | -1 (2.20956) | -1 | -1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11945.93958 HOMO: -7.18925 LUMO: 0.40001 factor:1 | -1 (2.07457) | 1 | 1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11945.70546 HOMO: -6.72121 LUMO: 0.19592 factor:1 | -1 (2.30870) | -1 | -1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11945.99104 HOMO: -6.85999 LUMO: -0.39457 factor:1 | -1 (2.02311) | -1 | -1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11946.21638 HOMO: -6.90625 LUMO: 0.05987 factor:1 | -1 (1.79777) | -1 | -1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11945.94758 HOMO: -7.00421 LUMO: 0.37552 factor:1 | -1 (2.06657) | -1 | -1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.71648 HOMO: -6.56883 LUMO: -0.97689 factor:1 | 1 (-0.70233) | -1 | -1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.18126 HOMO: -6.66679 LUMO: 0.56055 factor:1 | 1 (-0.16711) | -1 | -1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.14708 HOMO: -6.75931 LUMO: 0.32926 factor:1 | 1 (-0.13293) | -1 | -1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.78157 HOMO: -6.53617 LUMO: -1.06397 factor:1 | 1 (-0.76742) | -1 | -1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.17911 HOMO: -6.78108 LUMO: 0.42722 factor:1 | 1 (-0.16496) | -1 | -1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.98150 HOMO: -7.05319 LUMO: 0.61498 factor:1 | -1 (0.03265) | -1 | -1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.67754 HOMO: -6.78380 LUMO: 1.49391 factor:1 | 1 (-0.66339) | -1 | -1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.29971 HOMO: -7.21102 LUMO: 0.27211 factor:1 | 1 (-0.28556) | 1 | 1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.43345 HOMO: -6.67223 LUMO: 0.81362 factor:1 | 1 (-0.41930) | -1 | -1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.81970 HOMO: -6.69944 LUMO: 1.40683 factor:1 | -1 (0.19445) | -1 | -1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11945.35865 HOMO: -7.02598 LUMO: 1.46941 factor:1 | -1 (2.65550) | -1 | -1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11945.79417 HOMO: -5.85045 LUMO: -0.76736 factor:1 | -1 (2.21999) | -1 | -1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11945.93501 HOMO: -6.53890 LUMO: -0.50885 factor:1 | -1 (2.07914) | -1 | -1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11946.73108 HOMO: -6.42733 LUMO: -0.63947 factor:1 | -1 (1.28307) | -1 | -1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.20899 HOMO: -6.82189 LUMO: -0.85444 factor:1 | -1 (0.80516) | -1 | -1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11946.90251 HOMO: -6.97428 LUMO: -1.22179 factor:1 | -1 (1.11164) | -1 | -1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11946.46269 HOMO: -6.93346 LUMO: -1.09934 factor:1 | -1 (1.55146) | -1 | -1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11946.40237 HOMO: -7.17292 LUMO: -1.11839 factor:1 | -1 (1.61178) | 1 | 1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11946.74520 HOMO: -7.00965 LUMO: -1.23268 factor:1 | -1 (1.26895) | -1 | -1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11946.48229 HOMO: -6.73210 LUMO: -1.12383 factor:1 | -1 (1.53186) | -1 | -1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11946.38242 HOMO: -7.61375 LUMO: -0.11973 factor:1 | -1 (1.63173) | 1 | 1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11946.51562 HOMO: -7.42327 LUMO: 0.41906 factor:1 | -1 (1.49853) | 1 | 1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11946.77195 HOMO: -6.94162 LUMO: -1.01771 factor:1 | -1 (1.24220) | -1 | -1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.04932 HOMO: -6.82189 LUMO: -0.92791 factor:1 | -1 (0.96483) | -1 | -1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.05816 HOMO: -6.92258 LUMO: -1.73881 factor:1 | -1 (0.95599) | -1 | -1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.46252 HOMO: -6.50896 LUMO: -1.60819 factor:1 | -1 (0.55163) | -1 | -1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.34524 HOMO: -6.38379 LUMO: -2.18780 factor:1 | -1 (0.66891) | -1 | -1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.82323 HOMO: -6.48992 LUMO: -0.97417 factor:1 | 1 (-0.80908) | -1 | -1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.79928 HOMO: -6.01644 LUMO: -0.04354 factor:1 | 1 (-0.78513) | -1 | -1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.18009 HOMO: -6.70761 LUMO: -0.14422 factor:1 | 1 (-0.16594) | -1 | -1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.75207 HOMO: -6.70216 LUMO: 0.14422 factor:1 | 1 (-0.73792) | -1 | -1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.53914 HOMO: -7.07224 LUMO: -0.10885 factor:1 | 1 (-0.52499) | 1 | 1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.88742 HOMO: -7.52667 LUMO: -0.74287 factor:1 | 1 (-0.87327) | 1 | 1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.29769 HOMO: -6.48447 LUMO: -0.96056 factor:1 | 1 (-0.28354) | -1 | -1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.97301 HOMO: -6.22597 LUMO: -0.41361 factor:1 | -1 (0.04114) | -1 | -1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.49997 HOMO: -6.12256 LUMO: -1.05852 factor:1 | -1 (0.51419) | -1 | -1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.15947 HOMO: -6.97428 LUMO: -0.60681 factor:1 | -1 (0.85468) | -1 | -1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.74233 HOMO: -6.78380 LUMO: -0.88981 factor:1 | 1 (-0.72818) | -1 | -1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.15736 HOMO: -6.85999 LUMO: 0.07891 factor:1 | 1 (-1.14320) | -1 | -1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11946.89351 HOMO: -7.08312 LUMO: -0.60137 factor:1 | -1 (1.12065) | 1 | 1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11945.98745 HOMO: -6.57699 LUMO: -0.68028 factor:1 | -1 (2.02670) | -1 | -1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11945.86638 HOMO: -6.09807 LUMO: -0.31837 factor:1 | -1 (2.14777) | -1 | -1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11946.63089 HOMO: -6.10624 LUMO: 0.14966 factor:1 | -1 (1.38326) | -1 | -1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.48560 HOMO: -6.77019 LUMO: -0.95784 factor:1 | -1 (0.52855) | -1 | -1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11946.63252 HOMO: -5.93208 LUMO: -0.44627 factor:1 | -1 (1.38163) | -1 | -1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.74984 HOMO: -6.12256 LUMO: -0.27756 factor:1 | 1 (-0.73569) | -1 | -1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.11521 HOMO: -5.98106 LUMO: -0.37824 factor:1 | 1 (-1.10105) | -1 | -1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.95055 HOMO: -7.06408 LUMO: -1.12927 factor:1 | 1 (-0.93640) | 1 | 1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.44581 HOMO: -6.70761 LUMO: -0.98505 factor:1 | 1 (-0.43165) | -1 | -1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.03709 HOMO: -7.00965 LUMO: -0.42722 factor:1 | 1 (-0.02294) | -1 | -1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.21951 HOMO: -5.96201 LUMO: -0.59049 factor:1 | 1 (-1.20536) | -1 | -1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.76119 HOMO: -6.34570 LUMO: -1.68438 factor:1 | 1 (-0.74703) | -1 | -1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.28531 HOMO: -6.97156 LUMO: -1.85854 factor:1 | 1 (-0.27116) | -1 | -1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.78157 HOMO: -5.91848 LUMO: -2.51433 factor:1 | 1 (-0.76742) | -1 | -1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.45844 HOMO: -6.39195 LUMO: -1.66262 factor:1 | -1 (0.55571) | -1 | -1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.64636 HOMO: -6.50352 LUMO: 0.19592 factor:1 | -1 (0.36779) | -1 | -1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.30119 HOMO: -6.45998 LUMO: 0.34831 factor:1 | -1 (0.71297) | -1 | -1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.29983 HOMO: -7.05319 LUMO: 0.23402 factor:1 | -1 (0.71433) | -1 | -1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.49402 HOMO: -6.61237 LUMO: 0.18232 factor:1 | 1 (-0.47987) | -1 | -1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.85033 HOMO: -6.57427 LUMO: 0.40545 factor:1 | 1 (-0.83618) | -1 | -1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.30959 HOMO: -7.26544 LUMO: 0.41089 factor:1 | 1 (-0.29543) | 1 | 1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.46085 HOMO: -6.26406 LUMO: -0.85444 factor:1 | 1 (-0.44670) | -1 | -1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.09961 HOMO: -6.25318 LUMO: -0.79457 factor:1 | 1 (-1.08546) | -1 | -1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.29231 HOMO: -6.68040 LUMO: 0.41089 factor:1 | 1 (-0.27815) | -1 | -1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.85332 HOMO: -6.37835 LUMO: 0.37280 factor:1 | 1 (-0.83917) | -1 | -1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11946.89351 HOMO: -6.56067 LUMO: 0.62858 factor:1 | -1 (1.12065) | -1 | -1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11946.88063 HOMO: -6.74026 LUMO: -0.04082 factor:1 | -1 (1.13352) | -1 | -1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11946.57720 HOMO: -6.53617 LUMO: 0.35103 factor:1 | -1 (1.43695) | -1 | -1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11946.83037 HOMO: -6.51985 LUMO: 0.25851 factor:1 | -1 (1.18378) | -1 | -1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11946.87642 HOMO: -6.58788 LUMO: -1.98371 factor:1 | -1 (1.13774) | -1 | -1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.92470 HOMO: -6.51441 LUMO: 0.29116 factor:1 | 1 (-0.91055) | -1 | -1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.28700 HOMO: -6.81101 LUMO: 0.35647 factor:1 | 1 (-0.27285) | -1 | -1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.35742 HOMO: -6.42733 LUMO: 0.10340 factor:1 | 1 (-0.34327) | -1 | -1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.90396 HOMO: -6.70761 LUMO: 0.28028 factor:1 | 1 (-0.88981) | -1 | -1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.77335 HOMO: -6.67495 LUMO: 0.01633 factor:1 | 1 (-0.75920) | -1 | -1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.17799 HOMO: -6.75387 LUMO: 0.15510 factor:1 | 1 (-0.16384) | -1 | -1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.59857 HOMO: -6.56067 LUMO: 0.35919 factor:1 | 1 (-0.58442) | -1 | -1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.03140 HOMO: -7.16748 LUMO: 0.21497 factor:1 | 1 (-0.01725) | 1 | 1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.96432 HOMO: -6.71849 LUMO: 0.26667 factor:1 | 1 (-0.95017) | -1 | -1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.55673 HOMO: -6.69128 LUMO: 0.55783 factor:1 | -1 (0.45742) | -1 | -1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.11181 HOMO: -6.71305 LUMO: 0.45987 factor:1 | 1 (-0.09766) | -1 | -1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.08909 HOMO: -5.90487 LUMO: -0.70750 factor:1 | 1 (-0.07494) | -1 | -1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.50515 HOMO: -6.84638 LUMO: -0.72110 factor:1 | 1 (-0.49100) | -1 | -1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.49318 HOMO: -6.66135 LUMO: -1.13471 factor:1 | 1 (-0.47903) | -1 | -1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.19862 HOMO: -6.74026 LUMO: -0.64763 factor:1 | 1 (-0.18447) | -1 | -1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.62671 HOMO: -6.69672 LUMO: -1.05036 factor:1 | 1 (-0.61256) | -1 | -1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.68632 HOMO: -6.78924 LUMO: -1.03675 factor:1 | 1 (-1.67217) | -1 | -1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.79625 HOMO: -6.81373 LUMO: -0.85988 factor:1 | 1 (-1.78210) | -1 | -1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.11491 HOMO: -7.26544 LUMO: 0.91158 factor:1 | 1 (-1.10075) | 1 | 1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.66235 HOMO: -6.64230 LUMO: -1.92929 factor:1 | 1 (-1.64819) | -1 | -1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.79281 HOMO: -7.20830 LUMO: 0.11429 factor:1 | 1 (-0.77865) | 1 | 1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.50961 HOMO: -7.17020 LUMO: 0.04898 factor:1 | 1 (-1.49546) | 1 | 1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.05284 HOMO: -7.16476 LUMO: 0.04898 factor:1 | 1 (-1.03869) | 1 | 1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.94865 HOMO: -6.59332 LUMO: -0.49253 factor:1 | 1 (-0.93449) | -1 | -1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.75650 HOMO: -7.46953 LUMO: 0.84083 factor:1 | 1 (-1.74235) | 1 | 1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.10195 HOMO: -7.39878 LUMO: 0.88709 factor:1 | 1 (-1.08780) | 1 | 1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.14832 HOMO: -6.84094 LUMO: -0.61498 factor:1 | 1 (-1.13417) | -1 | -1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.12830 HOMO: -6.03549 LUMO: -0.27211 factor:1 | 1 (-0.11415) | -1 | -1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.19720 HOMO: -7.31170 LUMO: -0.64763 factor:1 | 1 (-0.18305) | 1 | 1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.21162 HOMO: -6.88992 LUMO: -0.84627 factor:1 | 1 (-0.19747) | -1 | -1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.65958 HOMO: -7.12666 LUMO: -0.09252 factor:1 | 1 (-0.64543) | 1 | 1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.32423 HOMO: -6.70489 LUMO: -0.63675 factor:1 | 1 (-0.31007) | -1 | -1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.13494 HOMO: -6.98788 LUMO: 0.86804 factor:1 | 1 (-0.12079) | -1 | -1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.99429 HOMO: -6.80285 LUMO: -0.60954 factor:1 | -1 (0.01986) | -1 | -1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.14585 HOMO: -7.02054 LUMO: -0.74287 factor:1 | 1 (-0.13170) | -1 | -1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.00253 HOMO: -7.03686 LUMO: -0.81090 factor:1 | -1 (0.01162) | -1 | -1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.39084 HOMO: -6.70489 LUMO: -1.00954 factor:1 | 1 (-0.37669) | -1 | -1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.73896 HOMO: -7.69810 LUMO: 0.00544 factor:1 | -1 (0.27519) | 1 | 1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11946.17646 HOMO: -6.83550 LUMO: -0.11157 factor:1 | -1 (1.83769) | -1 | -1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11946.15624 HOMO: -6.76203 LUMO: -2.13609 factor:1 | -1 (1.85791) | -1 | -1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11946.22310 HOMO: -6.72121 LUMO: -2.62862 factor:1 | -1 (1.79105) | -1 | -1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11946.85310 HOMO: -6.48719 LUMO: -2.73474 factor:1 | -1 (1.16106) | -1 | -1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.00069 HOMO: -6.83006 LUMO: -0.00544 factor:1 | -1 (1.01346) | -1 | -1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11946.49799 HOMO: -6.84094 LUMO: -1.11022 factor:1 | -1 (1.51616) | -1 | -1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11946.06383 HOMO: -6.66951 LUMO: -1.23812 factor:1 | -1 (1.95032) | -1 | -1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11946.26209 HOMO: -6.78380 LUMO: -1.27894 factor:1 | -1 (1.75206) | -1 | -1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.64541 HOMO: -6.50352 LUMO: -0.56055 factor:1 | -1 (0.36874) | -1 | -1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.84234 HOMO: -7.77974 LUMO: -0.26395 factor:1 | -1 (0.17181) | 1 | 1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.62933 HOMO: -7.01510 LUMO: -1.64085 factor:1 | -1 (0.38482) | -1 | -1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11946.15507 HOMO: -6.59876 LUMO: -0.91158 factor:1 | -1 (1.85908) | -1 | -1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11946.11012 HOMO: -4.67219 LUMO: -0.67756 factor:1 | -1 (1.90404) | -1 | -1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11946.16884 HOMO: -6.70489 LUMO: -0.65579 factor:1 | -1 (1.84531) | -1 | -1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11946.22525 HOMO: -6.62325 LUMO: -0.60409 factor:1 | -1 (1.78890) | -1 | -1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11946.80357 HOMO: -6.20147 LUMO: 0.15238 factor:1 | -1 (1.21058) | -1 | -1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11946.44686 HOMO: -6.43549 LUMO: -0.07075 factor:1 | -1 (1.56729) | -1 | -1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11946.45350 HOMO: -7.02054 LUMO: 0.13061 factor:1 | -1 (1.56065) | -1 | -1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11946.44863 HOMO: -7.04503 LUMO: 0.30749 factor:1 | -1 (1.56553) | -1 | -1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.11602 HOMO: -6.74842 LUMO: -0.99594 factor:1 | 1 (-1.10187) | -1 | -1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.16349 HOMO: -6.35658 LUMO: 0.41633 factor:1 | 1 (-0.14934) | -1 | -1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.43544 HOMO: -6.79740 LUMO: 0.56872 factor:1 | 1 (-0.42129) | -1 | -1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.71498 HOMO: -6.51713 LUMO: -0.05987 factor:1 | 1 (-0.70083) | -1 | -1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.16323 HOMO: -6.68040 LUMO: 0.34558 factor:1 | 1 (-2.14907) | -1 | -1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.23619 HOMO: -6.39740 LUMO: 0.50069 factor:1 | 1 (-1.22204) | -1 | -1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.09378 HOMO: -6.91713 LUMO: -0.97145 factor:1 | 1 (-2.07963) | -1 | -1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.48803 HOMO: -7.10761 LUMO: -0.27483 factor:1 | 1 (-1.47388) | 1 | -1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.72644 HOMO: -6.98788 LUMO: 0.40273 factor:1 | 1 (-0.71229) | -1 | -1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.12361 HOMO: -6.87087 LUMO: 0.28572 factor:1 | 1 (-1.10946) | -1 | -1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.08089 HOMO: -7.36612 LUMO: -0.12245 factor:1 | 1 (-1.06674) | 1 | 1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.77642 HOMO: -6.72938 LUMO: 0.33742 factor:1 | 1 (-1.76226) | -1 | -1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.69875 HOMO: -7.32531 LUMO: 0.07619 factor:1 | 1 (-1.68460) | 1 | 1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.97888 HOMO: -6.87087 LUMO: -0.08436 factor:1 | 1 (-0.96473) | -1 | -1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.86198 HOMO: -6.67495 LUMO: 0.85988 factor:1 | 1 (-0.84783) | -1 | -1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.10993 HOMO: -6.96339 LUMO: 0.65307 factor:1 | 1 (-1.09578) | -1 | -1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.62492 HOMO: -6.58516 LUMO: -0.78641 factor:1 | -1 (0.38923) | -1 | -1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.58503 HOMO: -6.56883 LUMO: 0.44355 factor:1 | -1 (0.42912) | -1 | -1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.59216 HOMO: -6.68312 LUMO: 0.43538 factor:1 | -1 (0.42199) | -1 | -1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.56116 HOMO: -6.81917 LUMO: 0.20681 factor:1 | -1 (0.45299) | -1 | -1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11946.82052 HOMO: -6.91169 LUMO: 0.08163 factor:1 | -1 (1.19363) | -1 | -1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11946.81734 HOMO: -4.88444 LUMO: -0.49253 factor:1 | -1 (1.19681) | -1 | -1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11946.86170 HOMO: -6.42189 LUMO: 0.64763 factor:1 | -1 (1.15246) | -1 | -1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.93674 HOMO: -6.24501 LUMO: 0.55783 factor:1 | -1 (0.07742) | -1 | -1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.59352 HOMO: -6.41372 LUMO: 0.29388 factor:1 | -1 (0.42063) | -1 | -1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.36130 HOMO: -5.67902 LUMO: 1.77690 factor:1 | -1 (0.65286) | -1 | -1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.42393 HOMO: -6.55794 LUMO: 0.05170 factor:1 | 1 (-0.40978) | -1 | -1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.69491 HOMO: -6.52801 LUMO: 0.25851 factor:1 | -1 (0.31924) | -1 | -1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.83918 HOMO: -7.08857 LUMO: 0.11157 factor:1 | -1 (0.17497) | 1 | 1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.40643 HOMO: -6.58243 LUMO: 0.75648 factor:1 | 1 (-0.39228) | -1 | -1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.76372 HOMO: -7.22190 LUMO: 0.45171 factor:1 | 1 (-0.74956) | 1 | 1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.62790 HOMO: -6.47087 LUMO: 0.00000 factor:1 | 1 (-0.61375) | -1 | -1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.61056 HOMO: -6.78652 LUMO: 1.32247 factor:1 | 1 (-1.59641) | -1 | -1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.85146 HOMO: -6.74026 LUMO: 1.45309 factor:1 | 1 (-1.83731) | -1 | -1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.14587 HOMO: -6.69944 LUMO: 0.76464 factor:1 | 1 (-1.13172) | -1 | -1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.55570 HOMO: -6.62325 LUMO: 0.64763 factor:1 | 1 (-1.54155) | -1 | -1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.67057 HOMO: -6.45182 LUMO: 0.49253 factor:1 | 1 (-0.65642) | -1 | -1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.50716 HOMO: -7.14843 LUMO: 0.62586 factor:1 | 1 (-1.49301) | 1 | 1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.78410 HOMO: -6.87087 LUMO: 1.53200 factor:1 | 1 (-0.76995) | -1 | -1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.54224 HOMO: -6.54978 LUMO: 0.45171 factor:1 | 1 (-0.52809) | -1 | -1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.90703 HOMO: -6.63686 LUMO: 0.80001 factor:1 | 1 (-1.89288) | -1 | -1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.21738 HOMO: -7.00693 LUMO: 1.56193 factor:1 | 1 (-1.20323) | -1 | -1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.92486 HOMO: -6.02460 LUMO: 1.72792 factor:1 | 1 (-0.91071) | -1 | -1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.94731 HOMO: -6.36746 LUMO: -1.20002 factor:1 | 1 (-0.93316) | -1 | -1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.11499 HOMO: -7.26816 LUMO: -1.06397 factor:1 | 1 (-1.10084) | 1 | 1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.82345 HOMO: -7.34707 LUMO: -1.09662 factor:1 | 1 (-0.80929) | 1 | 1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11945.84636 HOMO: -7.93212 LUMO: -0.13606 factor:1 | -1 (2.16780) | 1 | 1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11945.94146 HOMO: -6.80285 LUMO: 0.58504 factor:1 | -1 (2.07269) | -1 | -1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11945.90026 HOMO: -7.12938 LUMO: 0.32926 factor:1 | -1 (2.11389) | 1 | -1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11946.21929 HOMO: -6.86815 LUMO: -1.30070 factor:1 | -1 (1.79486) | -1 | -1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11946.95742 HOMO: -6.99333 LUMO: -1.03947 factor:1 | -1 (1.05673) | -1 | -1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11946.64387 HOMO: -7.56749 LUMO: -0.11157 factor:1 | -1 (1.37028) | 1 | 1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.15512 HOMO: -7.57293 LUMO: -0.07891 factor:1 | -1 (0.85904) | 1 | 1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11946.82082 HOMO: -7.30626 LUMO: 0.27211 factor:1 | -1 (1.19333) | 1 | 1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.45014 HOMO: -7.77974 LUMO: 0.27211 factor:1 | -1 (0.56401) | 1 | 1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.27504 HOMO: -7.11578 LUMO: 0.19864 factor:1 | -1 (0.73912) | 1 | 1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.20619 HOMO: -7.71171 LUMO: 0.57688 factor:1 | -1 (0.80796) | 1 | 1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11945.36110 HOMO: -7.83688 LUMO: 0.37824 factor:1 | -1 (2.65306) | 1 | 1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11945.89237 HOMO: -6.94979 LUMO: -1.66534 factor:1 | -1 (2.12178) | -1 | -1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11945.81852 HOMO: -6.97156 LUMO: -1.13199 factor:1 | -1 (2.19563) | -1 | -1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.19495 HOMO: -6.91441 LUMO: -1.08301 factor:1 | -1 (0.81920) | -1 | -1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11945.88217 HOMO: -6.71849 LUMO: -0.74831 factor:1 | -1 (2.13198) | -1 | -1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11945.86268 HOMO: -7.09401 LUMO: -1.77690 factor:1 | -1 (2.15147) | -1 | -1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11946.21385 HOMO: -6.97156 LUMO: -1.45037 factor:1 | -1 (1.80031) | -1 | -1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11946.21755 HOMO: -7.22462 LUMO: -1.11295 factor:1 | -1 (1.79660) | 1 | 1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11946.89038 HOMO: -7.85321 LUMO: 0.16599 factor:1 | -1 (1.12378) | 1 | 1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11946.74338 HOMO: -7.71987 LUMO: 0.55511 factor:1 | -1 (1.27077) | 1 | 1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11946.16628 HOMO: -7.63551 LUMO: 0.14422 factor:1 | -1 (1.84787) | 1 | 1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11946.45891 HOMO: -6.98788 LUMO: -0.80546 factor:1 | -1 (1.55524) | -1 | -1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11946.20552 HOMO: -6.98788 LUMO: -1.16737 factor:1 | -1 (1.80863) | -1 | -1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11946.48871 HOMO: -6.56611 LUMO: -1.60819 factor:1 | -1 (1.52544) | -1 | -1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.09090 HOMO: -6.95251 LUMO: 0.66396 factor:1 | -1 (0.92326) | -1 | -1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.29901 HOMO: -7.35252 LUMO: 0.49797 factor:1 | -1 (0.71514) | 1 | 1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.81150 HOMO: -6.90897 LUMO: -0.81090 factor:1 | 1 (-0.79735) | -1 | -1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.84062 HOMO: -7.04503 LUMO: -1.08301 factor:1 | 1 (-0.82646) | -1 | -1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.80803 HOMO: -6.92530 LUMO: -1.29526 factor:1 | -1 (0.20613) | -1 | -1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.12493 HOMO: -6.93074 LUMO: -1.25444 factor:1 | 1 (-0.11078) | -1 | -1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.95128 HOMO: -6.73482 LUMO: -0.62042 factor:1 | 1 (-0.93713) | -1 | -1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.32757 HOMO: -7.67633 LUMO: 0.59593 factor:1 | 1 (-0.31342) | 1 | 1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.88320 HOMO: -7.39061 LUMO: -0.19320 factor:1 | 1 (-0.86905) | 1 | 1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.85439 HOMO: -7.55388 LUMO: -0.20136 factor:1 | -1 (0.15976) | 1 | 1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.53607 HOMO: -7.14027 LUMO: -0.99866 factor:1 | 1 (-0.52191) | 1 | 1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.07107 HOMO: -6.75931 LUMO: -0.73199 factor:1 | 1 (-1.05692) | -1 | -1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.58973 HOMO: -5.45044 LUMO: -0.18776 factor:1 | 1 (-0.57558) | -1 | -1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11946.15488 HOMO: -6.70761 LUMO: -0.84083 factor:1 | -1 (1.85927) | -1 | -1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11946.50844 HOMO: -6.05453 LUMO: -1.06669 factor:1 | -1 (1.50571) | -1 | -1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11946.37007 HOMO: -6.86815 LUMO: -0.98233 factor:1 | -1 (1.64408) | -1 | -1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11946.46000 HOMO: -6.73210 LUMO: -0.95240 factor:1 | -1 (1.55415) | -1 | -1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11946.46123 HOMO: -5.89671 LUMO: -1.05036 factor:1 | -1 (1.55293) | -1 | -1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11945.14550 HOMO: -7.61102 LUMO: 0.33470 factor:1 | -1 (2.86865) | 1 | 1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.20475 HOMO: -7.51034 LUMO: 0.23674 factor:1 | -1 (0.80940) | 1 | 1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.23715 HOMO: -7.41510 LUMO: 0.62858 factor:1 | 1 (-0.22300) | 1 | 1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.66242 HOMO: -6.76203 LUMO: -1.72792 factor:1 | -1 (0.35173) | -1 | -1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.02554 HOMO: -6.60420 LUMO: -0.45715 factor:1 | 1 (-1.01139) | -1 | -1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.93036 HOMO: -6.59060 LUMO: -0.58232 factor:1 | 1 (-0.91621) | -1 | -1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.01363 HOMO: -7.43687 LUMO: -0.76736 factor:1 | 1 (-0.99947) | 1 | 1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.36912 HOMO: -6.08719 LUMO: -0.48708 factor:1 | 1 (-0.35497) | -1 | -1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.97041 HOMO: -5.88854 LUMO: -0.05714 factor:1 | 1 (-0.95626) | -1 | -1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.04613 HOMO: -7.34435 LUMO: -0.71838 factor:1 | 1 (-0.03197) | 1 | 1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.83338 HOMO: -7.46408 LUMO: -0.63130 factor:1 | 1 (-0.81923) | 1 | 1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.20980 HOMO: -7.00965 LUMO: -1.24900 factor:1 | 1 (-0.19565) | -1 | -1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.90343 HOMO: -6.91169 LUMO: -0.88981 factor:1 | -1 (0.11072) | -1 | -1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.11480 HOMO: -6.78652 LUMO: -0.82178 factor:1 | 1 (-1.10065) | -1 | -1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.50861 HOMO: -7.80423 LUMO: 0.87076 factor:1 | 1 (-0.49446) | 1 | 1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.05747 HOMO: -6.97700 LUMO: -1.00954 factor:1 | 1 (-0.04332) | -1 | -1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.03414 HOMO: -6.92530 LUMO: -0.88165 factor:1 | 1 (-1.01999) | -1 | -1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11946.59652 HOMO: -7.14571 LUMO: -1.04492 factor:1 | -1 (1.41763) | 1 | 1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11946.81957 HOMO: -7.49674 LUMO: 0.34558 factor:1 | -1 (1.19458) | 1 | 1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11946.91204 HOMO: -6.44094 LUMO: -1.20819 factor:1 | -1 (1.10212) | -1 | -1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.42249 HOMO: -6.47359 LUMO: -1.14016 factor:1 | -1 (0.59166) | -1 | -1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.47139 HOMO: -6.61237 LUMO: -0.87076 factor:1 | 1 (-2.45724) | -1 | -1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.77048 HOMO: -6.73754 LUMO: -1.09662 factor:1 | 1 (-1.75633) | -1 | -1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.67978 HOMO: -6.97700 LUMO: 0.13061 factor:1 | 1 (-2.66563) | -1 | -1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.41518 HOMO: -6.82734 LUMO: 0.59865 factor:1 | 1 (-2.40102) | -1 | -1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.44032 HOMO: -6.86543 LUMO: -0.91430 factor:1 | 1 (-2.42617) | -1 | -1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.83617 HOMO: -6.74298 LUMO: 0.28028 factor:1 | 1 (-1.82202) | -1 | -1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.52048 HOMO: -6.75387 LUMO: 0.19592 factor:1 | 1 (-2.50633) | -1 | -1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.83312 HOMO: -7.05591 LUMO: 0.10612 factor:1 | 1 (-2.81896) | -1 | -1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.45156 HOMO: -6.86543 LUMO: 0.49253 factor:1 | 1 (-2.43741) | -1 | -1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.43072 HOMO: -6.11440 LUMO: -1.12655 factor:1 | 1 (-1.41657) | -1 | -1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.66060 HOMO: -6.77291 LUMO: -1.02859 factor:1 | 1 (-1.64645) | -1 | -1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.21523 HOMO: -6.54978 LUMO: 0.29116 factor:1 | 1 (-2.20107) | -1 | -1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.21776 HOMO: -7.18108 LUMO: 0.00000 factor:1 | 1 (-2.20361) | 1 | 1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.33275 HOMO: -6.86271 LUMO: -1.15376 factor:1 | 1 (-2.31860) | -1 | -1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.71315 HOMO: -6.78108 LUMO: -1.22723 factor:1 | 1 (-1.69900) | -1 | -1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.38508 HOMO: -6.40828 LUMO: 0.02449 factor:1 | 1 (-2.37093) | -1 | -1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.18554 HOMO: -6.43821 LUMO: 0.09796 factor:1 | 1 (-2.17139) | -1 | -1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.71883 HOMO: -6.99877 LUMO: 0.40545 factor:1 | 1 (-2.70468) | -1 | -1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.73644 HOMO: -6.68856 LUMO: 0.19320 factor:1 | 1 (-1.72229) | -1 | -1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.47101 HOMO: -7.11034 LUMO: 0.31293 factor:1 | 1 (-2.45686) | 1 | 1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.52302 HOMO: -6.92530 LUMO: -0.85444 factor:1 | 1 (-1.50887) | -1 | -1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.01966 HOMO: -6.60148 LUMO: -0.59865 factor:1 | 1 (-2.00551) | -1 | -1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.40879 HOMO: -6.72938 LUMO: 0.30749 factor:1 | 1 (-1.39464) | -1 | -1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.22023 HOMO: -7.31170 LUMO: 0.06803 factor:1 | 1 (-2.20608) | 1 | 1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.33917 HOMO: -7.09129 LUMO: -0.04626 factor:1 | 1 (-2.32502) | 1 | 1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.31289 HOMO: -6.38379 LUMO: -0.76736 factor:1 | 1 (-2.29874) | -1 | -1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.99818 HOMO: -6.13617 LUMO: -0.63947 factor:1 | 1 (-2.98403) | -1 | -1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.17757 HOMO: -6.92258 LUMO: 0.37007 factor:1 | 1 (-2.16341) | -1 | -1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.11600 HOMO: -6.35930 LUMO: 0.41361 factor:1 | 1 (-0.10185) | -1 | -1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.41188 HOMO: -6.60420 LUMO: 0.26667 factor:1 | 1 (-2.39773) | -1 | -1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.79095 HOMO: -6.04909 LUMO: 1.82588 factor:1 | 1 (-1.77679) | -1 | -1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.45731 HOMO: -6.69672 LUMO: 1.72520 factor:1 | 1 (-1.44316) | -1 | -1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.03718 HOMO: -6.50080 LUMO: 0.29116 factor:1 | 1 (-2.02303) | -1 | -1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.87604 HOMO: -6.60692 LUMO: -0.43266 factor:1 | 1 (-1.86188) | -1 | -1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.06280 HOMO: -6.93890 LUMO: 0.39729 factor:1 | 1 (-1.04865) | -1 | -1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.05210 HOMO: -6.52801 LUMO: -0.47076 factor:1 | 1 (-1.03795) | -1 | -1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.92799 HOMO: -6.41100 LUMO: 0.30477 factor:1 | 1 (-0.91384) | -1 | -1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.97039 HOMO: -6.37291 LUMO: -0.80001 factor:1 | 1 (-0.95624) | -1 | -1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.86225 HOMO: -6.51985 LUMO: 1.44765 factor:1 | 1 (-0.84810) | -1 | -1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.40268 HOMO: -6.64774 LUMO: 0.04626 factor:1 | -1 (0.61147) | -1 | -1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.10530 HOMO: -6.65863 LUMO: 0.29933 factor:1 | 1 (-1.09115) | -1 | -1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.14403 HOMO: -7.09673 LUMO: 0.28300 factor:1 | 1 (-0.12988) | 1 | 1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.95814 HOMO: -6.57155 LUMO: -1.11567 factor:1 | 1 (-0.94399) | -1 | -1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.16255 HOMO: -6.38379 LUMO: -0.60681 factor:1 | 1 (-1.14840) | -1 | -1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.23044 HOMO: -6.60148 LUMO: 0.18232 factor:1 | 1 (-2.21629) | -1 | -1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.25030 HOMO: -6.96067 LUMO: -0.52246 factor:1 | 1 (-2.23615) | -1 | -1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.14976 HOMO: -6.57427 LUMO: -0.84627 factor:1 | 1 (-2.13560) | -1 | -1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.61526 HOMO: -6.59332 LUMO: -0.98233 factor:1 | 1 (-2.60111) | -1 | -1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.03843 HOMO: -6.20692 LUMO: -0.27483 factor:1 | 1 (-2.02428) | -1 | -1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.29896 HOMO: -6.81373 LUMO: 0.74559 factor:1 | 1 (-1.28481) | -1 | -1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.17642 HOMO: -6.60420 LUMO: 0.54695 factor:1 | 1 (-2.16227) | -1 | -1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.32938 HOMO: -6.58788 LUMO: -0.31021 factor:1 | 1 (-2.31523) | -1 | -1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.27768 HOMO: -6.72938 LUMO: 0.64763 factor:1 | 1 (-2.26352) | -1 | -1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.93008 HOMO: -6.86815 LUMO: 0.32109 factor:1 | 1 (-1.91593) | -1 | -1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.79699 HOMO: -6.63141 LUMO: 0.18776 factor:1 | 1 (-1.78284) | -1 | -1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.01398 HOMO: -7.18653 LUMO: 0.09524 factor:1 | 1 (-0.99983) | 1 | 1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.92029 HOMO: -6.83550 LUMO: 0.03537 factor:1 | 1 (-0.90614) | -1 | -1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.69046 HOMO: -7.47769 LUMO: 0.40817 factor:1 | 1 (-0.67631) | 1 | 1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.98720 HOMO: -6.57971 LUMO: -0.63675 factor:1 | 1 (-0.97305) | -1 | -1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.70272 HOMO: -6.74842 LUMO: -0.16327 factor:1 | 1 (-2.68857) | -1 | -1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.76185 HOMO: -7.07224 LUMO: 0.61770 factor:1 | 1 (-2.74770) | 1 | 1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.43191 HOMO: -6.83006 LUMO: 0.54695 factor:1 | 1 (-2.41776) | -1 | -1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.20538 HOMO: -6.60148 LUMO: 1.23540 factor:1 | 1 (-2.19122) | -1 | -1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.34686 HOMO: -6.99061 LUMO: 0.41089 factor:1 | 1 (-1.33270) | -1 | -1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.51573 HOMO: -6.63686 LUMO: 0.85172 factor:1 | 1 (-1.50158) | -1 | -1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.86036 HOMO: -6.50624 LUMO: 0.12517 factor:1 | 1 (-1.84621) | -1 | -1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.73789 HOMO: -6.35658 LUMO: 0.36463 factor:1 | 1 (-0.72374) | -1 | -1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.25422 HOMO: -6.34570 LUMO: 0.65035 factor:1 | 1 (-2.24007) | -1 | -1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.53530 HOMO: -6.63141 LUMO: 1.25717 factor:1 | 1 (-1.52114) | -1 | -1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.41562 HOMO: -6.91441 LUMO: 1.32792 factor:1 | 1 (-1.40147) | -1 | -1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.92640 HOMO: -7.15387 LUMO: 0.64219 factor:1 | 1 (-1.91225) | 1 | 1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.48507 HOMO: -7.17836 LUMO: 0.60409 factor:1 | 1 (-0.47092) | 1 | 1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.13448 HOMO: -6.92258 LUMO: 0.49525 factor:1 | 1 (-0.12033) | -1 | -1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.81390 HOMO: -6.31032 LUMO: 0.48708 factor:1 | -1 (0.20025) | -1 | -1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.24978 HOMO: -6.49808 LUMO: 0.31021 factor:1 | 1 (-0.23562) | -1 | -1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.86652 HOMO: -6.48447 LUMO: 0.37552 factor:1 | 1 (-0.85237) | -1 | -1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.07723 HOMO: -6.66135 LUMO: -1.08301 factor:1 | 1 (-0.06308) | -1 | -1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.90278 HOMO: -6.33481 LUMO: -0.51974 factor:1 | -1 (0.11138) | -1 | -1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.65664 HOMO: -6.76475 LUMO: -0.15238 factor:1 | 1 (-0.64249) | -1 | -1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.41435 HOMO: -6.93346 LUMO: -0.10885 factor:1 | 1 (-0.40020) | -1 | -1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.19630 HOMO: -7.19741 LUMO: 0.73199 factor:1 | 1 (-0.18215) | 1 | 1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.97254 HOMO: -6.82734 LUMO: 0.88437 factor:1 | 1 (-0.95839) | -1 | -1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.40290 HOMO: -7.01237 LUMO: 0.02721 factor:1 | 1 (-2.38875) | -1 | -1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.95838 HOMO: -6.39195 LUMO: 1.46941 factor:1 | 1 (-1.94423) | -1 | -1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.18989 HOMO: -6.53890 LUMO: 1.32792 factor:1 | 1 (-2.17574) | -1 | -1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.96585 HOMO: -6.82734 LUMO: 1.98099 factor:1 | 1 (-2.95170) | -1 | -1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11951.74802 HOMO: -6.74570 LUMO: 1.68983 factor:1 | 1 (-3.73386) | -1 | -1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.92613 HOMO: -6.41100 LUMO: 1.39050 factor:1 | 1 (-1.91198) | -1 | -1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.96016 HOMO: -5.92664 LUMO: 1.65989 factor:1 | 1 (-0.94600) | -1 | -1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.73700 HOMO: -6.07630 LUMO: 1.54833 factor:1 | 1 (-0.72284) | -1 | -1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.83634 HOMO: -6.45998 LUMO: 0.68573 factor:1 | 1 (-0.82219) | -1 | -1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.78837 HOMO: -6.52801 LUMO: 0.41361 factor:1 | 1 (-0.77422) | -1 | -1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.79153 HOMO: -6.77564 LUMO: 0.42178 factor:1 | 1 (-0.77737) | -1 | -1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.54023 HOMO: -6.56339 LUMO: 1.65717 factor:1 | 1 (-0.52608) | -1 | -1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.62935 HOMO: -5.85861 LUMO: 1.90752 factor:1 | 1 (-0.61520) | -1 | -1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.43601 HOMO: -6.77019 LUMO: -2.48440 factor:1 | 1 (-0.42186) | -1 | -1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.72102 HOMO: -6.53890 LUMO: -1.82588 factor:1 | 1 (-0.70687) | -1 | -1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.73577 HOMO: -6.50352 LUMO: -1.66806 factor:1 | 1 (-0.72162) | -1 | -1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.57509 HOMO: -6.90625 LUMO: 0.43538 factor:1 | 1 (-0.56094) | -1 | -1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.71196 HOMO: -6.85455 LUMO: 0.53062 factor:1 | 1 (-0.69781) | -1 | -1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.91958 HOMO: -6.49536 LUMO: 0.31021 factor:1 | 1 (-0.90543) | -1 | -1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.10465 HOMO: -4.97696 LUMO: -0.09252 factor:1 | 1 (-1.09050) | -1 | -1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.52733 HOMO: -5.31166 LUMO: 0.34286 factor:1 | 1 (-0.51318) | -1 | -1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.52611 HOMO: -6.42461 LUMO: 0.74287 factor:1 | 1 (-0.51196) | -1 | -1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.14406 HOMO: -6.59604 LUMO: 0.62858 factor:1 | 1 (-0.12991) | -1 | -1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.73914 HOMO: -6.45998 LUMO: -0.61770 factor:1 | 1 (-0.72499) | -1 | -1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.00709 HOMO: -6.75659 LUMO: -0.34014 factor:1 | 1 (-1.99293) | -1 | -1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.28696 HOMO: -6.63958 LUMO: 0.36191 factor:1 | 1 (-1.27281) | -1 | -1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.85073 HOMO: -5.92936 LUMO: -0.67484 factor:1 | 1 (-1.83658) | -1 | -1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.00728 HOMO: -5.67630 LUMO: 1.80956 factor:1 | 1 (-1.99313) | -1 | -1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.49917 HOMO: -6.50352 LUMO: -0.78369 factor:1 | 1 (-0.48502) | -1 | -1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.80432 HOMO: -6.35930 LUMO: -0.75648 factor:1 | 1 (-0.79016) | -1 | -1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.26520 HOMO: -6.74298 LUMO: 0.48980 factor:1 | 1 (-0.25105) | -1 | -1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.00196 HOMO: -6.85183 LUMO: 0.15510 factor:1 | -1 (0.01219) | -1 | -1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.64812 HOMO: -6.90897 LUMO: 0.26123 factor:1 | 1 (-0.63397) | -1 | -1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.30611 HOMO: -6.85999 LUMO: 0.47892 factor:1 | -1 (0.70804) | -1 | -1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.05797 HOMO: -6.69944 LUMO: 0.57416 factor:1 | -1 (0.95618) | -1 | -1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11946.79233 HOMO: -6.74026 LUMO: 0.69933 factor:1 | -1 (1.22182) | -1 | -1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.29478 HOMO: -6.52801 LUMO: 0.75376 factor:1 | 1 (-0.28063) | -1 | -1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.09309 HOMO: -7.05863 LUMO: 0.44627 factor:1 | 1 (-0.07894) | -1 | -1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.66769 HOMO: -6.96339 LUMO: 0.48164 factor:1 | 1 (-0.65354) | -1 | -1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.87078 HOMO: -6.95795 LUMO: 0.44355 factor:1 | -1 (0.14338) | -1 | -1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.11298 HOMO: -6.36746 LUMO: 0.58777 factor:1 | 1 (-0.09883) | -1 | -1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.52541 HOMO: -6.69400 LUMO: 0.40545 factor:1 | -1 (0.48874) | -1 | -1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.28926 HOMO: -6.30760 LUMO: -0.66668 factor:1 | 1 (-0.27511) | -1 | -1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.89565 HOMO: -6.53617 LUMO: -0.64491 factor:1 | -1 (0.11851) | -1 | -1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.36167 HOMO: -6.80829 LUMO: 0.17415 factor:1 | 1 (-0.34752) | -1 | -1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.88623 HOMO: -6.80285 LUMO: 0.73471 factor:1 | -1 (0.12792) | -1 | -1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.54102 HOMO: -6.43821 LUMO: 0.21769 factor:1 | 1 (-0.52687) | -1 | -1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.38877 HOMO: -6.98788 LUMO: 0.10885 factor:1 | 1 (-0.37462) | -1 | -1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11946.04780 HOMO: -7.15115 LUMO: 0.40817 factor:1 | -1 (1.96635) | 1 | 1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11945.89702 HOMO: -6.00011 LUMO: -0.98505 factor:1 | -1 (2.11713) | -1 | -1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11946.47355 HOMO: -6.16882 LUMO: -0.77825 factor:1 | -1 (1.54060) | -1 | -1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.02722 HOMO: -6.30760 LUMO: 0.34831 factor:1 | -1 (0.98693) | -1 | -1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11946.55641 HOMO: -6.64502 LUMO: 0.63403 factor:1 | -1 (1.45774) | -1 | -1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11946.96836 HOMO: -6.93618 LUMO: 0.96600 factor:1 | -1 (1.04579) | -1 | -1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11946.70869 HOMO: -6.45182 LUMO: 0.16327 factor:1 | -1 (1.30547) | -1 | -1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11946.77152 HOMO: -6.99605 LUMO: 0.20953 factor:1 | -1 (1.24264) | -1 | -1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11946.81582 HOMO: -6.72665 LUMO: 0.32654 factor:1 | -1 (1.19834) | -1 | -1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11946.28326 HOMO: -6.38379 LUMO: 0.45443 factor:1 | -1 (1.73089) | -1 | -1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11945.80864 HOMO: -6.65318 LUMO: 0.04354 factor:1 | -1 (2.20551) | -1 | -1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11946.00598 HOMO: -6.94707 LUMO: -1.68438 factor:1 | -1 (2.00817) | -1 | -1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11945.90709 HOMO: -6.71849 LUMO: 0.15783 factor:1 | -1 (2.10706) | -1 | -1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11946.03324 HOMO: -6.97156 LUMO: 0.43266 factor:1 | -1 (1.98091) | -1 | -1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11946.08799 HOMO: -6.91441 LUMO: -0.54695 factor:1 | -1 (1.92616) | -1 | -1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11946.12802 HOMO: -6.74842 LUMO: -0.76192 factor:1 | -1 (1.88613) | -1 | -1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11945.63887 HOMO: -6.70489 LUMO: 0.19048 factor:1 | -1 (2.37528) | -1 | -1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11945.72537 HOMO: -7.25728 LUMO: 0.33470 factor:1 | -1 (2.28878) | 1 | -1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11945.88881 HOMO: -6.96339 LUMO: 0.55511 factor:1 | -1 (2.12535) | -1 | -1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11945.74557 HOMO: -6.77564 LUMO: 0.72382 factor:1 | -1 (2.26859) | -1 | -1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.24078 HOMO: -6.75387 LUMO: 0.39729 factor:1 | -1 (0.77337) | -1 | -1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.82704 HOMO: -7.00149 LUMO: 0.06531 factor:1 | 1 (-0.81289) | -1 | -1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.56140 HOMO: -7.09945 LUMO: 0.33470 factor:1 | 1 (-0.54725) | 1 | 1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.74431 HOMO: -7.20830 LUMO: 0.59593 factor:1 | 1 (-0.73016) | 1 | 1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.15674 HOMO: -6.40556 LUMO: 0.56600 factor:1 | 1 (-0.14259) | -1 | -1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.14308 HOMO: -6.77291 LUMO: 0.73471 factor:1 | 1 (-0.12893) | -1 | -1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.72576 HOMO: -6.65046 LUMO: 0.09796 factor:1 | 1 (-0.71160) | -1 | -1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.13024 HOMO: -6.95795 LUMO: 0.22313 factor:1 | 1 (-0.11608) | -1 | -1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.89395 HOMO: -6.85727 LUMO: 0.04626 factor:1 | 1 (-0.87980) | -1 | -1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.55550 HOMO: -7.27360 LUMO: 0.42178 factor:1 | 1 (-0.54134) | 1 | 1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.88261 HOMO: -6.78924 LUMO: -0.13334 factor:1 | -1 (0.13154) | -1 | -1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.98744 HOMO: -6.63141 LUMO: 0.38368 factor:1 | 1 (-1.97329) | -1 | -1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.05469 HOMO: -6.92258 LUMO: 0.39184 factor:1 | 1 (-1.04054) | -1 | -1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.61667 HOMO: -6.19331 LUMO: -0.46804 factor:1 | 1 (-0.60251) | -1 | -1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.44185 HOMO: -7.26544 LUMO: -0.05442 factor:1 | 1 (-1.42770) | 1 | 1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.90290 HOMO: -7.09401 LUMO: 0.30749 factor:1 | 1 (-0.88875) | 1 | 1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.68064 HOMO: -6.14705 LUMO: -0.88709 factor:1 | 1 (-0.66649) | -1 | -1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.62605 HOMO: -6.53617 LUMO: -0.28572 factor:1 | 1 (-1.61189) | -1 | -1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.83695 HOMO: -6.37291 LUMO: -0.67212 factor:1 | -1 (0.17720) | -1 | -1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.56242 HOMO: -6.65591 LUMO: 0.03810 factor:1 | -1 (0.45174) | -1 | -1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.94568 HOMO: -7.11034 LUMO: 0.75103 factor:1 | 1 (-0.93153) | 1 | 1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.69163 HOMO: -6.85183 LUMO: -0.05987 factor:1 | 1 (-0.67748) | -1 | -1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.97616 HOMO: -6.70761 LUMO: -0.05442 factor:1 | -1 (0.03799) | -1 | -1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.16528 HOMO: -6.23413 LUMO: 0.06259 factor:1 | 1 (-0.15113) | -1 | -1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.10425 HOMO: -6.55794 LUMO: 0.74015 factor:1 | 1 (-0.09010) | -1 | -1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.27950 HOMO: -7.27905 LUMO: 0.26939 factor:1 | -1 (0.73465) | 1 | 1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.49689 HOMO: -6.34842 LUMO: -0.86804 factor:1 | -1 (0.51726) | -1 | -1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.39798 HOMO: -6.27222 LUMO: 1.46125 factor:1 | -1 (0.61617) | -1 | -1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.27603 HOMO: -6.65046 LUMO: 2.04902 factor:1 | 1 (-0.26188) | -1 | -1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.46133 HOMO: -7.11850 LUMO: -1.14016 factor:1 | -1 (0.55283) | 1 | -1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.22203 HOMO: -6.88720 LUMO: -1.20274 factor:1 | -1 (0.79212) | -1 | -1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11946.90757 HOMO: -6.69400 LUMO: -0.31565 factor:1 | -1 (1.10658) | -1 | -1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.00401 HOMO: -6.95523 LUMO: -1.55377 factor:1 | -1 (1.01014) | -1 | -1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11946.61957 HOMO: -6.41372 LUMO: -0.83539 factor:1 | -1 (1.39458) | -1 | -1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.29808 HOMO: -6.13889 LUMO: -0.90070 factor:1 | 1 (-0.28392) | -1 | -1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.32613 HOMO: -6.44366 LUMO: -0.55511 factor:1 | 1 (-0.31198) | -1 | -1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.83901 HOMO: -6.10079 LUMO: -0.71022 factor:1 | 1 (-0.82486) | -1 | -1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.43492 HOMO: -6.90353 LUMO: -0.64763 factor:1 | 1 (-0.42077) | -1 | -1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.92922 HOMO: -6.65046 LUMO: -0.82450 factor:1 | 1 (-0.91506) | -1 | -1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.15233 HOMO: -6.81645 LUMO: -0.85444 factor:1 | 1 (-0.13818) | -1 | -1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11946.46871 HOMO: -6.20692 LUMO: 1.30887 factor:1 | -1 (1.54544) | -1 | -1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11946.39135 HOMO: -5.96201 LUMO: 1.33880 factor:1 | -1 (1.62281) | -1 | -1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11946.66398 HOMO: -6.52529 LUMO: 1.58914 factor:1 | -1 (1.35017) | -1 | -1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11945.55568 HOMO: -6.58516 LUMO: 1.97555 factor:1 | -1 (2.45847) | -1 | -1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11945.39285 HOMO: -6.84366 LUMO: 0.15783 factor:1 | -1 (2.62130) | -1 | -1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11945.86633 HOMO: -6.45726 LUMO: 0.42994 factor:1 | -1 (2.14782) | -1 | -1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11945.64156 HOMO: -6.75387 LUMO: 0.14422 factor:1 | -1 (2.37259) | -1 | -1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.21841 HOMO: -6.69944 LUMO: 1.79051 factor:1 | -1 (0.79574) | -1 | -1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11946.56833 HOMO: -6.59876 LUMO: 1.90208 factor:1 | -1 (1.44582) | -1 | -1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.22538 HOMO: -7.05863 LUMO: 1.20819 factor:1 | -1 (0.78878) | -1 | -1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11946.45176 HOMO: -6.54978 LUMO: 2.01636 factor:1 | -1 (1.56240) | -1 | -1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.31952 HOMO: -5.52119 LUMO: 1.95106 factor:1 | 1 (-0.30537) | -1 | -1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.47683 HOMO: -6.53617 LUMO: 1.60275 factor:1 | 1 (-0.46268) | -1 | -1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.20643 HOMO: -6.11440 LUMO: 1.89119 factor:1 | 1 (-0.19228) | -1 | -1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.15464 HOMO: -7.31986 LUMO: 0.48708 factor:1 | 1 (-0.14049) | 1 | 1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.63258 HOMO: -6.76475 LUMO: -0.75648 factor:1 | 1 (-0.61843) | -1 | -1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.09451 HOMO: -6.76747 LUMO: -1.06941 factor:1 | 1 (-0.08036) | -1 | -1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.82577 HOMO: -6.87087 LUMO: 0.72927 factor:1 | -1 (0.18838) | -1 | -1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11946.44623 HOMO: -7.00965 LUMO: 0.02177 factor:1 | -1 (1.56792) | -1 | -1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11946.46484 HOMO: -6.54706 LUMO: -0.03265 factor:1 | -1 (1.54931) | -1 | -1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11946.66205 HOMO: -6.62325 LUMO: -0.63675 factor:1 | -1 (1.35211) | -1 | -1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11946.67543 HOMO: -7.03414 LUMO: -1.24084 factor:1 | -1 (1.33872) | -1 | -1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11946.66074 HOMO: -7.04503 LUMO: -0.10068 factor:1 | -1 (1.35341) | -1 | -1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.42176 HOMO: -6.67223 LUMO: 0.03537 factor:1 | -1 (0.59239) | -1 | -1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.43724 HOMO: -6.82734 LUMO: 0.58777 factor:1 | -1 (0.57691) | -1 | -1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.58500 HOMO: -6.84366 LUMO: 0.46531 factor:1 | -1 (0.42915) | -1 | -1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.54042 HOMO: -7.03959 LUMO: -1.15104 factor:1 | 1 (-0.52627) | -1 | -1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.51278 HOMO: -6.91169 LUMO: -0.41361 factor:1 | -1 (0.50137) | -1 | -1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.62214 HOMO: -7.10217 LUMO: -0.44627 factor:1 | -1 (0.39201) | 1 | 1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.08124 HOMO: -6.88176 LUMO: -0.19592 factor:1 | -1 (0.93292) | -1 | -1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.46339 HOMO: -7.21374 LUMO: -0.46531 factor:1 | -1 (0.55076) | 1 | 1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.48266 HOMO: -6.54978 LUMO: 0.16871 factor:1 | -1 (0.53149) | -1 | -1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.94224 HOMO: -6.71305 LUMO: -0.13061 factor:1 | 1 (-1.92809) | -1 | -1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.29023 HOMO: -6.74842 LUMO: -0.36191 factor:1 | 1 (-1.27608) | -1 | -1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.37535 HOMO: -6.74570 LUMO: -0.09796 factor:1 | 1 (-1.36120) | -1 | -1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.62328 HOMO: -6.93890 LUMO: -0.27211 factor:1 | 1 (-0.60913) | -1 | -1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.40983 HOMO: -6.88720 LUMO: -0.18776 factor:1 | 1 (-0.39568) | -1 | -1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.60369 HOMO: -6.74842 LUMO: 0.02993 factor:1 | 1 (-0.58953) | -1 | -1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.77712 HOMO: -6.70216 LUMO: 0.01361 factor:1 | 1 (-1.76297) | -1 | -1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.04280 HOMO: -6.90625 LUMO: 0.00544 factor:1 | 1 (-1.02864) | -1 | -1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.81093 HOMO: -6.18243 LUMO: 0.25851 factor:1 | 1 (-0.79678) | -1 | -1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.06272 HOMO: -6.32937 LUMO: -0.20953 factor:1 | 1 (-1.04856) | -1 | -1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.81106 HOMO: -6.78108 LUMO: 0.00544 factor:1 | 1 (-0.79691) | -1 | -1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11946.77075 HOMO: -5.97562 LUMO: 0.28572 factor:1 | -1 (1.24340) | -1 | -1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11946.30794 HOMO: -5.97290 LUMO: -0.18504 factor:1 | -1 (1.70621) | -1 | -1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11946.56825 HOMO: -6.12800 LUMO: 0.42178 factor:1 | -1 (1.44590) | -1 | -1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11946.85982 HOMO: -6.24229 LUMO: -0.00816 factor:1 | -1 (1.15433) | -1 | -1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11946.53421 HOMO: -6.61781 LUMO: 0.12789 factor:1 | -1 (1.47995) | -1 | -1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.29623 HOMO: -6.70489 LUMO: 0.14694 factor:1 | -1 (0.71792) | -1 | -1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.77112 HOMO: -6.86543 LUMO: -0.21225 factor:1 | 1 (-0.75697) | -1 | -1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.51313 HOMO: -6.90081 LUMO: -0.20136 factor:1 | 1 (-0.49898) | -1 | -1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.26588 HOMO: -7.12938 LUMO: -0.25851 factor:1 | 1 (-0.25173) | 1 | 1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.57808 HOMO: -6.93074 LUMO: -0.26667 factor:1 | 1 (-0.56393) | -1 | -1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.61097 HOMO: -7.00421 LUMO: -0.31021 factor:1 | 1 (-1.59682) | -1 | -1 |
| G: -5683.64846 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.33306 HOMO: -7.10761 LUMO: -0.17415 factor:1 | 1 (-1.31891) | 1 | 1 |
| G: -5683.64846 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.50414 HOMO: -8.21240 LUMO: 0.05987 factor:1 | 1 (-1.48999) | 1 | 1 |
| G: -5683.64846 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.79958 HOMO: -7.14843 LUMO: -0.46531 factor:1 | 1 (-0.78543) | 1 | -1 |
| G: -5683.64846 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.53302 HOMO: -6.80829 LUMO: -0.29933 factor:1 | 1 (-0.51887) | -1 | -1 |
| G: -5683.64846 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.09153 HOMO: -6.84094 LUMO: -0.53606 factor:1 | 1 (-1.07738) | -1 | -1 |
| G: -5683.64846 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.68637 HOMO: -6.81917 LUMO: -0.26667 factor:1 | 1 (-1.67222) | -1 | -1 |
| G: -5683.64846 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.00429 HOMO: -6.85727 LUMO: -1.20002 factor:1 | 1 (-0.99014) | -1 | -1 |
| G: -5683.64846 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.63620 HOMO: -6.39468 LUMO: -1.06941 factor:1 | 1 (-0.62205) | -1 | -1 |
| G: -5683.64846 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.67797 HOMO: -6.00827 LUMO: -1.94017 factor:1 | 1 (-0.66382) | -1 | -1 |
| G: -5683.64846 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.55553 HOMO: -6.80829 LUMO: 0.18504 factor:1 | -1 (0.45862) | -1 | -1 |
| G: -5683.64846 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.69483 HOMO: -6.54434 LUMO: -0.95784 factor:1 | -1 (0.31933) | -1 | -1 |
| G: -5683.64846 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.75626 HOMO: -6.45454 LUMO: -0.07347 factor:1 | 1 (-0.74211) | -1 | -1 |
| G: -5683.64846 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.23081 HOMO: -5.33887 LUMO: 1.11839 factor:1 | 1 (-0.21666) | -1 | -1 |
| G: -5683.64846 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.52047 HOMO: -5.75249 LUMO: 0.70477 factor:1 | 1 (-0.50632) | -1 | -1 |
| G: -5683.64846 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.85254 HOMO: -5.64092 LUMO: 0.87076 factor:1 | -1 (0.16161) | -1 | -1 |
| G: -5683.64846 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.41604 HOMO: -5.14295 LUMO: 1.06124 factor:1 | 1 (-0.40188) | -1 | -1 |
| G: -5683.64846 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.62366 HOMO: -5.05043 LUMO: 1.21091 factor:1 | 1 (-0.60951) | -1 | -1 |
| G: -5683.64846 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.49686 HOMO: -5.05588 LUMO: 1.02859 factor:1 | 1 (-2.48271) | -1 | -1 |
| G: -5683.64846 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11951.00011 HOMO: -5.76337 LUMO: 0.79457 factor:1 | 1 (-2.98596) | -1 | -1 |
| G: -5683.64846 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.03411 HOMO: -5.01506 LUMO: 1.00138 factor:1 | 1 (-2.01996) | -1 | -1 |
| G: -5683.64846 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.14497 HOMO: -4.84363 LUMO: 1.53744 factor:1 | 1 (-2.13081) | -1 | -1 |
| G: -5683.64846 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.04491 HOMO: -5.17833 LUMO: 1.45309 factor:1 | 1 (-2.03076) | -1 | -1 |
| G: -5683.64846 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.08097 HOMO: -5.13751 LUMO: 0.51157 factor:1 | 1 (-2.06681) | -1 | -1 |
| G: -5683.64846 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.08900 HOMO: -5.56473 LUMO: 0.32109 factor:1 | 1 (-1.07485) | -1 | -1 |
| G: -5683.64846 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.65938 HOMO: -4.69941 LUMO: 1.14016 factor:1 | 1 (-1.64523) | -1 | -1 |
| G: -5683.64846 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.81286 HOMO: -4.49260 LUMO: 1.86398 factor:1 | 1 (-0.79871) | -1 | -1 |
| G: -5683.64846 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.61927 HOMO: -4.32117 LUMO: 1.68438 factor:1 | 1 (-1.60512) | -1 | -1 |
| G: -5683.64846 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.73807 HOMO: -4.44906 LUMO: 1.37690 factor:1 | 1 (-1.72392) | -1 | -1 |
| G: -5683.64846 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.72989 HOMO: -4.62049 LUMO: 1.34968 factor:1 | 1 (-0.71574) | -1 | -1 |
| G: -5683.64846 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.83070 HOMO: -4.59600 LUMO: 1.58370 factor:1 | 1 (-1.81655) | -1 | -1 |
| G: -5683.64846 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.43545 HOMO: -4.98785 LUMO: 1.46669 factor:1 | 1 (-2.42130) | -1 | -1 |
| G: -5683.64846 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.57894 HOMO: -5.06676 LUMO: 1.27349 factor:1 | 1 (-1.56479) | -1 | -1 |
| G: -5683.64846 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.79658 HOMO: -5.09125 LUMO: 1.13471 factor:1 | 1 (-1.78243) | -1 | -1 |
| G: -5683.64846 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.96448 HOMO: -4.84635 LUMO: 1.33608 factor:1 | 1 (-0.95033) | -1 | -1 |
| G: -5683.64846 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.09326 HOMO: -4.94431 LUMO: 1.18370 factor:1 | 1 (-2.07911) | -1 | -1 |
| G: -5683.64846 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.44599 HOMO: -4.92526 LUMO: 1.39867 factor:1 | 1 (-1.43184) | -1 | -1 |
| G: -5683.64846 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.78042 HOMO: -5.71983 LUMO: 0.60137 factor:1 | 1 (-0.76627) | -1 | -1 |
| G: -5683.64846 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.12829 HOMO: -5.10486 LUMO: 1.05580 factor:1 | 1 (-2.11413) | -1 | -1 |
| G: -5683.64846 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.76120 HOMO: -5.20282 LUMO: 1.01226 factor:1 | 1 (-2.74704) | -1 | -1 |
| G: -5683.64846 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.55290 HOMO: -4.98513 LUMO: 1.53744 factor:1 | 1 (-1.53875) | -1 | -1 |
| G: -5683.64846 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.47793 HOMO: -5.67085 LUMO: 0.17687 factor:1 | 1 (-2.46377) | -1 | -1 |
| G: -5683.64846 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.86855 HOMO: -5.87222 LUMO: 0.12517 factor:1 | 1 (-1.85440) | -1 | -1 |
| G: -5683.64846 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.77794 HOMO: -5.20826 LUMO: 0.91702 factor:1 | 1 (-1.76379) | -1 | -1 |
| G: -5683.64846 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.99169 HOMO: -5.94569 LUMO: 0.63130 factor:1 | 1 (-0.97754) | -1 | -1 |
| G: -5683.64846 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.42213 HOMO: -5.35792 LUMO: 0.91430 factor:1 | 1 (-0.40798) | -1 | -1 |
| G: -5683.64846 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.02821 HOMO: -5.36336 LUMO: 1.44220 factor:1 | 1 (-1.01406) | -1 | -1 |
| G: -5683.64846 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.00966 HOMO: -5.83412 LUMO: 0.71294 factor:1 | -1 (0.00449) | -1 | -1 |
| G: -5683.64846 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.20022 HOMO: -4.97696 LUMO: 1.72792 factor:1 | 1 (-0.18607) | -1 | -1 |
| G: -5683.64846 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.07390 HOMO: -5.55929 LUMO: 0.23130 factor:1 | 1 (-1.05975) | -1 | -1 |
| G: -5683.64846 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.50409 HOMO: -5.71167 LUMO: 0.47348 factor:1 | 1 (-0.48994) | -1 | -1 |
| G: -5683.64846 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.40203 HOMO: -7.31986 LUMO: -2.54699 factor:1 | 1 (-2.38788) | -1 | -1 |
| G: -5683.64846 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.99653 HOMO: -5.34704 LUMO: 1.19730 factor:1 | 1 (-1.98238) | -1 | -1 |
| G: -5683.64846 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.39537 HOMO: -5.45860 LUMO: 0.80818 factor:1 | 1 (-1.38122) | -1 | -1 |
| G: -5683.64846 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.67173 HOMO: -5.12663 LUMO: 1.20274 factor:1 | 1 (-1.65758) | -1 | -1 |
| G: -5683.64846 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.06103 HOMO: -5.37153 LUMO: 1.05580 factor:1 | 1 (-1.04688) | -1 | -1 |
| G: -5683.64846 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.57018 HOMO: -5.47221 LUMO: 0.97961 factor:1 | 1 (-1.55603) | -1 | -1 |
| G: -5683.64846 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.67440 HOMO: -5.06948 LUMO: 1.12111 factor:1 | 1 (-1.66025) | -1 | -1 |
| G: -5683.64846 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.67226 HOMO: -5.19737 LUMO: 1.25444 factor:1 | 1 (-0.65811) | -1 | -1 |
| G: -5683.64846 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.82679 HOMO: -5.27901 LUMO: 1.00682 factor:1 | 1 (-0.81264) | -1 | -1 |
| G: -5683.64846 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.10443 HOMO: -5.38513 LUMO: 0.49253 factor:1 | 1 (-1.09028) | -1 | -1 |
| G: -5683.64846 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.79838 HOMO: -5.12390 LUMO: 1.22995 factor:1 | 1 (-0.78423) | -1 | -1 |
| G: -5683.64846 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.88690 HOMO: -5.31438 LUMO: 0.70205 factor:1 | 1 (-0.87275) | -1 | -1 |
| G: -5683.64846 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.00568 HOMO: -5.17561 LUMO: 1.04492 factor:1 | 1 (-0.99153) | -1 | -1 |
| G: -5683.64846 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.75693 HOMO: -4.94431 LUMO: 1.52656 factor:1 | 1 (-1.74278) | -1 | -1 |
| G: -5683.64846 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.11483 HOMO: -5.13751 LUMO: 0.93879 factor:1 | 1 (-1.10067) | -1 | -1 |
| G: -5683.64846 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.83982 HOMO: -5.49942 LUMO: 0.97689 factor:1 | 1 (-1.82567) | -1 | -1 |
| G: -5683.64846 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.42143 HOMO: -5.79058 LUMO: 0.53879 factor:1 | 1 (-2.40728) | -1 | -1 |
| G: -5683.64846 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.51632 HOMO: -5.36881 LUMO: 1.56465 factor:1 | 1 (-2.50217) | -1 | -1 |
| G: -5683.64846 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.82816 HOMO: -4.67492 LUMO: 1.32792 factor:1 | 1 (-2.81401) | -1 | -1 |
| G: -5683.64846 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.03492 HOMO: -4.60145 LUMO: 1.19458 factor:1 | 1 (-2.02077) | -1 | -1 |
| G: -5683.64846 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.78186 HOMO: -4.49260 LUMO: 1.60547 factor:1 | 1 (-1.76771) | -1 | -1 |
| G: -5683.64846 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.30853 HOMO: -4.65043 LUMO: 1.34696 factor:1 | 1 (-2.29438) | -1 | -1 |
| G: -5683.64846 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.89717 HOMO: -4.77560 LUMO: 1.35241 factor:1 | 1 (-2.88302) | -1 | -1 |
| G: -5683.64846 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11951.66091 HOMO: -4.94431 LUMO: 1.17825 factor:1 | 1 (-3.64676) | -1 | -1 |
| G: -5683.64846 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.88210 HOMO: -4.87084 LUMO: 1.41771 factor:1 | 1 (-2.86794) | -1 | -1 |
| G: -5683.64846 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11951.03429 HOMO: -5.34432 LUMO: 1.16737 factor:1 | 1 (-3.02014) | -1 | -1 |
| G: -5683.64846 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.33400 HOMO: -4.94975 LUMO: 1.67622 factor:1 | 1 (-2.31985) | -1 | -1 |
| G: -5683.64846 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.94169 HOMO: -4.81369 LUMO: 1.14288 factor:1 | 1 (-2.92754) | -1 | -1 |
| G: -5683.64846 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.54644 HOMO: -5.22459 LUMO: 0.29660 factor:1 | 1 (-2.53229) | -1 | -1 |
| G: -5683.64846 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.65540 HOMO: -5.21642 LUMO: 0.37824 factor:1 | 1 (-2.64125) | -1 | -1 |
| G: -5683.64846 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.05626 HOMO: -5.00417 LUMO: 1.01226 factor:1 | 1 (-2.04211) | -1 | -1 |
| G: -5683.64846 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.34133 HOMO: -5.46677 LUMO: 0.10612 factor:1 | 1 (-1.32718) | -1 | -1 |
| G: -5683.64846 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.24089 HOMO: -5.51303 LUMO: 0.54151 factor:1 | 1 (-2.22673) | -1 | -1 |
| G: -5683.64846 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.19357 HOMO: -5.63004 LUMO: 0.17960 factor:1 | 1 (-2.17941) | -1 | -1 |
| G: -5683.64846 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.40367 HOMO: -4.79193 LUMO: 1.12111 factor:1 | 1 (-1.38952) | -1 | -1 |
| G: -5683.64846 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.49227 HOMO: -5.43411 LUMO: 0.45987 factor:1 | 1 (-1.47812) | -1 | -1 |
| G: -5683.64846 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.38996 HOMO: -7.06135 LUMO: -2.13881 factor:1 | 1 (-1.37581) | 1 | 1 |
| G: -5683.64846 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.72777 HOMO: -5.33071 LUMO: 1.14016 factor:1 | 1 (-0.71362) | -1 | -1 |
| G: -5683.64846 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.84179 HOMO: -7.12394 LUMO: -0.03810 factor:1 | 1 (-0.82763) | 1 | 1 |
| G: -5683.64846 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.76668 HOMO: -7.20558 LUMO: -2.50889 factor:1 | 1 (-0.75253) | 1 | 1 |
| G: -5683.64846 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.87964 HOMO: -7.26816 LUMO: -2.11432 factor:1 | 1 (-0.86549) | 1 | 1 |
| G: -5683.64846 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.06031 HOMO: -7.89674 LUMO: 0.31021 factor:1 | -1 (0.95384) | 1 | 1 |
| G: -5683.64846 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.92214 HOMO: -7.26544 LUMO: 0.22858 factor:1 | 1 (-0.90799) | 1 | 1 |
| G: -5683.64846 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.70426 HOMO: -7.12666 LUMO: -0.02449 factor:1 | 1 (-0.69011) | 1 | 1 |
| G: -5683.64846 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.84739 HOMO: -7.68722 LUMO: 0.71838 factor:1 | 1 (-0.83324) | 1 | 1 |
| G: -5683.64846 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.97930 HOMO: -6.86271 LUMO: -0.96056 factor:1 | 1 (-1.96515) | -1 | -1 |
| G: -5683.64846 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.38843 HOMO: -7.07496 LUMO: -1.11839 factor:1 | 1 (-2.37428) | 1 | 1 |
| G: -5683.64846 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.93237 HOMO: -7.06952 LUMO: -2.08439 factor:1 | 1 (-0.91822) | 1 | 1 |
| G: -5683.64846 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.66214 HOMO: -6.60965 LUMO: -2.11977 factor:1 | 1 (-0.64798) | -1 | -1 |
| G: -5683.64846 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.91001 HOMO: -6.87360 LUMO: -1.85854 factor:1 | 1 (-0.89585) | -1 | -1 |
| G: -5683.64846 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.37686 HOMO: -7.67089 LUMO: -0.24762 factor:1 | 1 (-2.36271) | 1 | 1 |
| G: -5683.64846 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.02499 HOMO: -6.45726 LUMO: -1.86398 factor:1 | 1 (-2.01084) | -1 | -1 |
| G: -5683.64846 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.74726 HOMO: -6.91713 LUMO: 0.33198 factor:1 | -1 (0.26689) | -1 | -1 |
| G: -5683.64846 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.61451 HOMO: -6.83278 LUMO: 0.26667 factor:1 | 1 (-1.60036) | -1 | -1 |
| G: -5683.64846 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.77340 HOMO: -6.89264 LUMO: -1.00682 factor:1 | 1 (-1.75924) | -1 | -1 |
| G: -5683.64846 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.88500 HOMO: -6.57427 LUMO: 0.22041 factor:1 | 1 (-0.87085) | -1 | -1 |
| G: -5683.64846 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.88960 HOMO: -7.52123 LUMO: -0.01905 factor:1 | 1 (-0.87544) | 1 | 1 |
| G: -5683.64846 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.53539 HOMO: -7.37429 LUMO: -0.08980 factor:1 | 1 (-0.52123) | 1 | 1 |
| G: -5683.64846 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.89205 HOMO: -7.28449 LUMO: -0.26395 factor:1 | 1 (-0.87789) | 1 | 1 |
| G: -5683.64846 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.07243 HOMO: -6.79740 LUMO: -0.60954 factor:1 | 1 (-1.05828) | -1 | -1 |
| G: -5683.64846 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.74148 HOMO: -7.12666 LUMO: -0.60681 factor:1 | 1 (-0.72733) | 1 | 1 |
| G: -5683.64846 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.74880 HOMO: -6.96611 LUMO: -0.30477 factor:1 | 1 (-0.73465) | -1 | -1 |
| G: -5683.64846 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.74290 HOMO: -7.08040 LUMO: -0.31293 factor:1 | 1 (-0.72875) | 1 | 1 |
| G: -5683.64846 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.51348 HOMO: -6.78924 LUMO: -0.73743 factor:1 | 1 (-0.49933) | -1 | -1 |
| G: -5683.64846 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.55258 HOMO: -7.57293 LUMO: -1.11295 factor:1 | 1 (-0.53843) | 1 | 1 |
| G: -5683.64846 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.19220 HOMO: -7.15932 LUMO: -0.23130 factor:1 | 1 (-0.17804) | 1 | 1 |
| G: -5683.64846 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.67245 HOMO: -7.48585 LUMO: -0.10068 factor:1 | 1 (-0.65830) | 1 | 1 |
| G: -5683.64846 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.05596 HOMO: -7.17020 LUMO: -0.26123 factor:1 | -1 (0.95819) | 1 | 1 |
| G: -5683.64846 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11945.77784 HOMO: -7.43143 LUMO: -0.16055 factor:1 | -1 (2.23631) | 1 | 1 |
| G: -5683.64846 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11946.05520 HOMO: -7.14843 LUMO: -0.10612 factor:1 | -1 (1.95895) | 1 | 1 |
| G: -5683.64846 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.07399 HOMO: -6.95523 LUMO: -0.22585 factor:1 | 1 (-0.05984) | -1 | -1 |
| G: -5683.64846 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.67310 HOMO: -7.06680 LUMO: -0.51974 factor:1 | 1 (-0.65895) | 1 | 1 |
| G: -5683.64846 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.34240 HOMO: -6.80829 LUMO: -0.64763 factor:1 | 1 (-0.32825) | -1 | -1 |
| G: -5683.64846 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.94445 HOMO: -7.13210 LUMO: -0.48164 factor:1 | 1 (-0.93030) | 1 | 1 |
| G: -5683.64846 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.27818 HOMO: -7.16204 LUMO: -0.45715 factor:1 | 1 (-0.26403) | 1 | 1 |
| G: -5683.64846 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11946.77846 HOMO: -7.15115 LUMO: -0.43266 factor:1 | -1 (1.23570) | 1 | 1 |
| G: -5683.64846 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11946.80594 HOMO: -7.15932 LUMO: -2.52794 factor:1 | -1 (1.20821) | -1 | -1 |
| G: -5683.64846 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11946.78270 HOMO: -7.21102 LUMO: -2.65311 factor:1 | -1 (1.23145) | -1 | -1 |
| G: -5683.64846 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.47762 HOMO: -6.57427 LUMO: -2.78645 factor:1 | 1 (-0.46346) | -1 | -1 |
| G: -5683.64846 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.72649 HOMO: -6.40828 LUMO: -3.23815 factor:1 | 1 (-0.71234) | -1 | -1 |
| G: -5683.64846 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.11496 HOMO: -7.71987 LUMO: -0.20953 factor:1 | 1 (-1.10081) | 1 | 1 |
| G: -5683.64846 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.08585 HOMO: -7.47769 LUMO: -0.43810 factor:1 | 1 (-1.07169) | 1 | 1 |
| G: -5683.64846 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.43416 HOMO: -6.68040 LUMO: -2.22589 factor:1 | 1 (-0.42001) | -1 | -1 |
| G: -5683.64846 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.77330 HOMO: -6.92802 LUMO: -1.99187 factor:1 | 1 (-0.75914) | -1 | -1 |
| G: -5683.64846 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.77370 HOMO: -7.73620 LUMO: 0.01633 factor:1 | 1 (-0.75955) | 1 | 1 |
| G: -5683.64846 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.10860 HOMO: -7.28721 LUMO: -0.18504 factor:1 | 1 (-0.09445) | 1 | 1 |
| G: -5683.64846 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.92849 HOMO: -7.49674 LUMO: -0.19864 factor:1 | -1 (0.08566) | 1 | 1 |
| G: -5683.64846 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.97792 HOMO: -7.10489 LUMO: -2.56331 factor:1 | 1 (-0.96377) | -1 | -1 |
| G: -5683.64846 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.34774 HOMO: -7.36612 LUMO: 0.16055 factor:1 | 1 (-0.33358) | 1 | 1 |
| G: -5683.64846 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.26809 HOMO: -7.67633 LUMO: 0.33198 factor:1 | 1 (-0.25394) | 1 | 1 |
| G: -5683.64846 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.42036 HOMO: -7.07768 LUMO: -0.27483 factor:1 | 1 (-0.40621) | 1 | 1 |
| G: -5683.64846 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.56676 HOMO: -7.32531 LUMO: 0.05442 factor:1 | 1 (-0.55261) | 1 | 1 |
| G: -5683.64846 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.71599 HOMO: -6.79740 LUMO: -1.21635 factor:1 | 1 (-0.70184) | -1 | -1 |
| G: -5683.64846 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.21904 HOMO: -7.14027 LUMO: 0.12517 factor:1 | 1 (-1.20489) | 1 | -1 |
| G: -5683.64846 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.87172 HOMO: -7.17292 LUMO: 0.16871 factor:1 | 1 (-0.85757) | 1 | -1 |
| G: -5683.64846 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.68437 HOMO: -7.08312 LUMO: -1.38778 factor:1 | 1 (-0.67022) | 1 | 1 |
| G: -5683.64846 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.68801 HOMO: -6.75387 LUMO: -1.88031 factor:1 | 1 (-0.67386) | -1 | -1 |
| G: -5683.64846 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.65465 HOMO: -7.07768 LUMO: -1.25717 factor:1 | 1 (-0.64050) | 1 | 1 |
| G: -5683.64846 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.40844 HOMO: -6.46543 LUMO: -1.14016 factor:1 | 1 (-0.39429) | -1 | -1 |
| G: -5683.64846 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.54355 HOMO: -7.37973 LUMO: -0.45987 factor:1 | 1 (-0.52940) | 1 | 1 |
| G: -5683.64846 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11946.86311 HOMO: -7.46408 LUMO: 0.03265 factor:1 | -1 (1.15104) | 1 | 1 |
| G: -5683.64846 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.99472 HOMO: -7.96477 LUMO: -0.19864 factor:1 | -1 (0.01943) | 1 | 1 |
| G: -5683.64846 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.35900 HOMO: -6.93890 LUMO: -1.11839 factor:1 | 1 (-0.34485) | -1 | -1 |
| G: -5683.64846 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.76301 HOMO: -7.06408 LUMO: -1.08846 factor:1 | 1 (-0.74886) | 1 | 1 |
| G: -5683.64846 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.68310 HOMO: -7.14027 LUMO: -0.33470 factor:1 | -1 (0.33105) | 1 | 1 |
| G: -5683.64846 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.82049 HOMO: -7.38245 LUMO: 0.10885 factor:1 | -1 (0.19366) | 1 | 1 |
| G: -5683.64846 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.88174 HOMO: -7.59470 LUMO: -1.21363 factor:1 | -1 (0.13241) | 1 | 1 |
| G: -5683.64846 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.93376 HOMO: -7.23279 LUMO: -1.23812 factor:1 | 1 (-0.91961) | 1 | 1 |
| G: -5683.64846 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.89467 HOMO: -6.90897 LUMO: 0.23402 factor:1 | -1 (0.11949) | -1 | -1 |
| G: -5683.64846 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.23334 HOMO: -7.36340 LUMO: -0.17143 factor:1 | 1 (-0.21919) | 1 | 1 |
| G: -5683.64846 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.28692 HOMO: -6.61781 LUMO: -0.01361 factor:1 | 1 (-0.27277) | -1 | -1 |
| G: -5683.64846 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11943.79832 HOMO: -6.80013 LUMO: 0.38368 factor:1 | -1 (4.21583) | -1 | -1 |
| G: -5683.64846 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.24730 HOMO: -6.72121 LUMO: -0.95512 factor:1 | 1 (-0.23315) | -1 | -1 |
| G: -5683.64846 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.83600 HOMO: -6.24773 LUMO: -0.69933 factor:1 | -1 (0.17815) | -1 | -1 |
| G: -5683.64846 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.36905 HOMO: -6.56883 LUMO: 0.14694 factor:1 | -1 (0.64510) | -1 | -1 |
| G: -5683.64846 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.40228 HOMO: -6.51441 LUMO: -1.27621 factor:1 | -1 (0.61188) | -1 | -1 |
| G: -5683.64846 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.00302 HOMO: -6.91986 LUMO: -1.16737 factor:1 | -1 (0.01113) | -1 | -1 |
| G: -5683.64846 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.48043 HOMO: -6.17971 LUMO: -0.65307 factor:1 | -1 (0.53372) | -1 | -1 |
| G: -5683.64846 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.87264 HOMO: -7.22462 LUMO: 0.04354 factor:1 | 1 (-0.85849) | 1 | 1 |
| G: -5683.64846 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.91624 HOMO: -7.16204 LUMO: -0.23674 factor:1 | 1 (-0.90208) | 1 | 1 |
| G: -5683.64846 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.28583 HOMO: -6.81645 LUMO: -0.19320 factor:1 | 1 (-0.27168) | -1 | -1 |
| G: -5683.64846 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.82848 HOMO: -6.69400 LUMO: 0.04082 factor:1 | 1 (-0.81433) | -1 | -1 |
| G: -5683.64846 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.10594 HOMO: -6.63141 LUMO: -0.22858 factor:1 | 1 (-0.09178) | -1 | -1 |
| G: -5683.64846 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.33876 HOMO: -6.92258 LUMO: -1.11295 factor:1 | 1 (-0.32460) | -1 | -1 |
| G: -5683.64846 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.94279 HOMO: -6.60148 LUMO: -1.13744 factor:1 | 1 (-0.92864) | -1 | -1 |
| G: -5683.64846 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.33190 HOMO: -6.78108 LUMO: -0.82450 factor:1 | 1 (-0.31775) | -1 | -1 |
| G: -5683.64846 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.83145 HOMO: -7.05591 LUMO: -0.97145 factor:1 | -1 (0.18270) | -1 | -1 |
| G: -5683.64846 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.44496 HOMO: -6.65318 LUMO: -1.26261 factor:1 | 1 (-0.43081) | -1 | -1 |
| G: -5683.64846 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11946.98510 HOMO: -6.98244 LUMO: -0.98233 factor:1 | -1 (1.02905) | -1 | -1 |
| G: -5683.64846 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11946.85051 HOMO: -7.11850 LUMO: -0.99594 factor:1 | -1 (1.16364) | 1 | 1 |
| G: -5683.64846 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11946.85323 HOMO: -6.64230 LUMO: -0.93879 factor:1 | -1 (1.16092) | -1 | -1 |
| G: -5683.64846 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11946.30509 HOMO: -6.62053 LUMO: -1.22451 factor:1 | -1 (1.70907) | -1 | -1 |
| G: -5683.64846 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11946.40180 HOMO: -7.02598 LUMO: -0.85172 factor:1 | -1 (1.61236) | -1 | -1 |
| G: -5683.64846 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.62350 HOMO: -7.06680 LUMO: -0.89253 factor:1 | 1 (-0.60934) | 1 | 1 |
| G: -5683.64846 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.83645 HOMO: -7.17292 LUMO: 0.00272 factor:1 | 1 (-0.82230) | 1 | 1 |
| G: -5683.64846 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.69697 HOMO: -7.03142 LUMO: -0.35103 factor:1 | 1 (-0.68282) | -1 | -1 |
| G: -5683.64846 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.77784 HOMO: -6.96884 LUMO: -0.09796 factor:1 | 1 (-0.76369) | -1 | -1 |
| G: -5683.64846 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.13992 HOMO: -6.56339 LUMO: -0.99322 factor:1 | 1 (-0.12577) | -1 | -1 |
| G: -5683.64846 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.70334 HOMO: -7.08857 LUMO: -0.17687 factor:1 | -1 (0.31081) | 1 | 1 |
| G: -5683.64846 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.69131 HOMO: -7.05863 LUMO: -0.22041 factor:1 | 1 (-0.67716) | -1 | -1 |
| G: -5683.64846 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.96669 HOMO: -7.15115 LUMO: -0.17960 factor:1 | 1 (-0.95253) | 1 | 1 |
| G: -5683.64846 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.34050 HOMO: -6.67495 LUMO: -0.96600 factor:1 | 1 (-0.32635) | -1 | -1 |
| G: -5683.64846 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.87360 HOMO: -6.74026 LUMO: -1.79867 factor:1 | -1 (0.14055) | -1 | -1 |
| G: -5683.64846 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.70868 HOMO: -6.73482 LUMO: -1.78235 factor:1 | -1 (0.30548) | -1 | -1 |
| G: -5683.64846 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.59240 HOMO: -6.09807 LUMO: 0.16871 factor:1 | -1 (0.42175) | -1 | -1 |
| G: -5683.64846 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.94566 HOMO: -6.72393 LUMO: 0.27211 factor:1 | -1 (0.06849) | -1 | -1 |
| G: -5683.64846 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.77918 HOMO: -6.40556 LUMO: -0.04354 factor:1 | -1 (0.23497) | -1 | -1 |
| G: -5683.64846 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.13543 HOMO: -6.56883 LUMO: 0.22041 factor:1 | 1 (-0.12128) | -1 | -1 |
| G: -5683.64846 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.30948 HOMO: -7.22462 LUMO: 0.15783 factor:1 | 1 (-0.29533) | 1 | 1 |
| G: -5683.64846 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.59848 HOMO: -6.83550 LUMO: 0.19320 factor:1 | 1 (-1.58433) | -1 | -1 |
| G: -5683.64846 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.76987 HOMO: -7.26816 LUMO: -0.07619 factor:1 | 1 (-0.75571) | 1 | -1 |
| G: -5683.64846 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.53217 HOMO: -7.13483 LUMO: 0.33198 factor:1 | 1 (-0.51802) | 1 | 1 |
| G: -5683.64846 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.49484 HOMO: -6.58243 LUMO: -0.26395 factor:1 | 1 (-0.48069) | -1 | -1 |
| G: -5683.64846 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.14367 HOMO: -7.38517 LUMO: 0.17143 factor:1 | 1 (-1.12952) | 1 | 1 |
| G: -5683.64846 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.93368 HOMO: -6.80013 LUMO: 0.25851 factor:1 | 1 (-0.91953) | -1 | -1 |
| G: -5683.64846 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.78034 HOMO: -6.96611 LUMO: 0.11429 factor:1 | 1 (-0.76619) | -1 | -1 |
| G: -5683.64846 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.85175 HOMO: -6.51713 LUMO: -1.14560 factor:1 | 1 (-0.83759) | -1 | -1 |
| G: -5683.64846 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.36298 HOMO: -7.15387 LUMO: -0.35647 factor:1 | -1 (0.65117) | 1 | 1 |
| G: -5683.64846 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.32320 HOMO: -5.26540 LUMO: 1.26805 factor:1 | -1 (0.69095) | -1 | -1 |
| G: -5683.64846 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.61177 HOMO: -6.76475 LUMO: -0.16327 factor:1 | 1 (-0.59762) | -1 | -1 |
| G: -5683.64846 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.84788 HOMO: -6.55250 LUMO: -0.71838 factor:1 | 1 (-0.83373) | -1 | -1 |
| G: -5683.64846 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.25870 HOMO: -6.76203 LUMO: -1.08301 factor:1 | 1 (-0.24455) | -1 | -1 |
| G: -5683.64846 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.77046 HOMO: -7.14027 LUMO: -0.01633 factor:1 | 1 (-1.75630) | 1 | 1 |
| G: -5683.64846 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.65255 HOMO: -6.94979 LUMO: -0.93879 factor:1 | 1 (-1.63840) | -1 | -1 |
| G: -5683.64846 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.86558 HOMO: -6.74842 LUMO: 0.31293 factor:1 | -1 (0.14857) | -1 | -1 |
| G: -5683.64846 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.03089 HOMO: -6.43821 LUMO: 0.05987 factor:1 | 1 (-0.01674) | -1 | -1 |
| G: -5683.64846 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.54950 HOMO: -6.60420 LUMO: 0.22585 factor:1 | 1 (-1.53535) | -1 | -1 |
| G: -5683.64846 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.90382 HOMO: -6.43821 LUMO: 0.05987 factor:1 | 1 (-1.88967) | -1 | -1 |
| G: -5683.64846 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.47331 HOMO: -6.34570 LUMO: 1.43948 factor:1 | 1 (-1.45916) | -1 | -1 |
| G: -5683.64846 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.16608 HOMO: -6.03004 LUMO: 1.21363 factor:1 | 1 (-2.15193) | -1 | -1 |
| G: -5683.64846 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.88949 HOMO: -6.68040 LUMO: -0.92247 factor:1 | 1 (-0.87534) | -1 | -1 |
| G: -5683.64846 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.87575 HOMO: -6.92530 LUMO: -0.31293 factor:1 | 1 (-0.86159) | -1 | -1 |
| G: -5683.64846 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.74297 HOMO: -6.94979 LUMO: -0.19864 factor:1 | 1 (-1.72882) | -1 | -1 |
| G: -5683.64846 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.84276 HOMO: -6.80829 LUMO: -0.30477 factor:1 | 1 (-1.82861) | -1 | -1 |
| G: -5683.64846 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.76551 HOMO: -7.22734 LUMO: -1.02859 factor:1 | 1 (-0.75136) | 1 | 1 |
| G: -5683.64846 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.77659 HOMO: -6.93890 LUMO: -0.72382 factor:1 | 1 (-0.76244) | -1 | -1 |
| G: -5683.64846 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.42435 HOMO: -7.27088 LUMO: -0.78097 factor:1 | 1 (-2.41019) | 1 | 1 |
| G: -5683.64846 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.90578 HOMO: -7.29809 LUMO: -0.97145 factor:1 | 1 (-1.89163) | 1 | 1 |
| G: -5683.64846 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.97822 HOMO: -7.18925 LUMO: -0.94696 factor:1 | 1 (-1.96406) | 1 | 1 |
| G: -5683.64846 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.28938 HOMO: -7.33891 LUMO: -0.96873 factor:1 | 1 (-2.27523) | 1 | 1 |
| G: -5683.64846 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.68665 HOMO: -7.36068 LUMO: -0.28028 factor:1 | 1 (-0.67250) | 1 | 1 |
| G: -5683.64846 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.79708 HOMO: -7.10761 LUMO: -1.14832 factor:1 | 1 (-0.78293) | 1 | 1 |
| G: -5683.64846 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.68057 HOMO: -6.94707 LUMO: -0.65307 factor:1 | 1 (-2.66642) | -1 | -1 |
| G: -5683.64846 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.97424 HOMO: -6.91713 LUMO: -1.81228 factor:1 | 1 (-1.96009) | -1 | -1 |
| G: -5683.64846 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.66077 HOMO: -6.78652 LUMO: -2.01636 factor:1 | 1 (-1.64662) | -1 | -1 |
| G: -5683.64846 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.74631 HOMO: -6.52801 LUMO: -1.17553 factor:1 | 1 (-2.73216) | -1 | -1 |
| G: -5683.64846 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.86708 HOMO: -7.54844 LUMO: -1.18642 factor:1 | 1 (-1.85293) | 1 | -1 |
| G: -5683.64846 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.15436 HOMO: -7.52939 LUMO: -1.23812 factor:1 | 1 (-1.14021) | 1 | -1 |
| G: -5683.64846 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.07580 HOMO: -7.94572 LUMO: -0.81634 factor:1 | 1 (-2.06164) | 1 | 1 |
| G: -5683.64846 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.38596 HOMO: -7.55932 LUMO: -0.86260 factor:1 | 1 (-1.37181) | 1 | 1 |
| G: -5683.64846 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.41216 HOMO: -7.72259 LUMO: -1.39050 factor:1 | 1 (-1.39801) | 1 | -1 |
| G: -5683.64846 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.40591 HOMO: -7.11850 LUMO: -1.01498 factor:1 | 1 (-1.39175) | 1 | -1 |
| G: -5683.64846 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.52044 HOMO: -7.09673 LUMO: -1.00954 factor:1 | 1 (-1.50629) | 1 | -1 |
| G: -5683.64846 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.54550 HOMO: -6.06270 LUMO: 0.16327 factor:1 | 1 (-1.53135) | -1 | -1 |
| G: -5683.64846 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.50281 HOMO: -5.71167 LUMO: 0.70477 factor:1 | 1 (-1.48865) | -1 | -1 |
| G: -5683.64846 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.11834 HOMO: -5.38241 LUMO: 0.86260 factor:1 | 1 (-1.10418) | -1 | -1 |
| G: -5683.64846 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.48553 HOMO: -5.67357 LUMO: 1.27621 factor:1 | 1 (-1.47137) | -1 | -1 |
| G: -5683.64846 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.44969 HOMO: -7.56204 LUMO: -0.68573 factor:1 | 1 (-1.43554) | 1 | 1 |
| G: -5683.64846 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.29627 HOMO: -5.57833 LUMO: 1.13199 factor:1 | 1 (-1.28212) | -1 | -1 |
| G: -5683.64846 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.70624 HOMO: -7.58653 LUMO: -0.66124 factor:1 | 1 (-1.69209) | 1 | 1 |
| G: -5683.64846 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.73493 HOMO: -7.91851 LUMO: -1.10206 factor:1 | 1 (-0.72078) | 1 | -1 |
| G: -5683.64846 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.67895 HOMO: -6.48992 LUMO: -1.00138 factor:1 | 1 (-0.66480) | -1 | -1 |
| G: -5683.64846 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.80957 HOMO: -7.09673 LUMO: -0.45171 factor:1 | 1 (-0.79542) | 1 | 1 |
| G: -5683.64846 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.66173 HOMO: -6.63686 LUMO: 0.09252 factor:1 | 1 (-0.64758) | -1 | -1 |
| G: -5683.64846 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.56641 HOMO: -6.84366 LUMO: -0.14422 factor:1 | 1 (-0.55226) | -1 | -1 |
| G: -5683.64846 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.80105 HOMO: -6.93074 LUMO: 0.04354 factor:1 | 1 (-0.78690) | -1 | -1 |
| G: -5683.64846 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.03054 HOMO: -6.90353 LUMO: -0.19864 factor:1 | -1 (0.98361) | -1 | -1 |
| G: -5683.64846 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.54573 HOMO: -6.59876 LUMO: -0.10068 factor:1 | 1 (-0.53157) | -1 | -1 |
| G: -5683.64846 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.62714 HOMO: -6.74570 LUMO: -0.44627 factor:1 | 1 (-0.61299) | -1 | -1 |
| G: -5683.64846 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.69329 HOMO: -6.60148 LUMO: -0.61770 factor:1 | 1 (-0.67914) | -1 | -1 |
| G: -5683.64846 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.39600 HOMO: -6.55794 LUMO: -1.06941 factor:1 | 1 (-1.38185) | -1 | -1 |
| G: -5683.64846 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.73631 HOMO: -7.12666 LUMO: -0.11973 factor:1 | 1 (-1.72215) | 1 | 1 |
| G: -5683.64846 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.58928 HOMO: -7.21646 LUMO: -0.50069 factor:1 | 1 (-1.57513) | 1 | 1 |
| G: -5683.64846 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.89310 HOMO: -7.27632 LUMO: -1.00682 factor:1 | 1 (-1.87895) | 1 | -1 |
| G: -5683.64846 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.37233 HOMO: -6.74298 LUMO: 0.04354 factor:1 | 1 (-1.35817) | -1 | -1 |
| G: -5683.64846 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.39396 HOMO: -6.37291 LUMO: 0.14150 factor:1 | 1 (-1.37981) | -1 | -1 |
| G: -5683.64846 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.06625 HOMO: -5.61371 LUMO: 1.28438 factor:1 | 1 (-1.05210) | -1 | -1 |
| G: -5683.64846 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.08919 HOMO: -5.52119 LUMO: 0.99866 factor:1 | 1 (-1.07504) | -1 | -1 |
| G: -5683.64846 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.50090 HOMO: -6.51985 LUMO: -0.10885 factor:1 | 1 (-1.48675) | -1 | -1 |
| G: -5683.64846 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.30846 HOMO: -5.61371 LUMO: 0.77280 factor:1 | 1 (-1.29431) | -1 | -1 |
| G: -5683.64846 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.28174 HOMO: -5.58922 LUMO: 0.24490 factor:1 | 1 (-1.26759) | -1 | -1 |
| G: -5683.64846 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.43967 HOMO: -6.32665 LUMO: -0.57144 factor:1 | 1 (-1.42552) | -1 | -1 |
| G: -5683.64846 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.13134 HOMO: -6.29127 LUMO: -0.93607 factor:1 | 1 (-1.11719) | -1 | -1 |
| G: -5683.64846 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.93333 HOMO: -5.49670 LUMO: 0.27211 factor:1 | -1 (0.08082) | -1 | -1 |
| G: -5683.64846 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.96163 HOMO: -5.68990 LUMO: 0.24218 factor:1 | -1 (0.05252) | -1 | -1 |
| G: -5683.64846 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.01260 HOMO: -5.68174 LUMO: 0.69933 factor:1 | -1 (0.00155) | -1 | -1 |
| G: -5683.64846 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.09430 HOMO: -5.28173 LUMO: 1.00954 factor:1 | 1 (-2.08015) | -1 | -1 |
| G: -5683.64846 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.82370 HOMO: -5.94025 LUMO: 0.73471 factor:1 | 1 (-2.80955) | -1 | -1 |
| G: -5683.64846 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.14278 HOMO: -5.65725 LUMO: 1.28710 factor:1 | 1 (-0.12863) | -1 | -1 |
| G: -5683.64846 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.18359 HOMO: -5.41507 LUMO: 0.87076 factor:1 | 1 (-1.16944) | -1 | -1 |
| G: -5683.64846 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.83381 HOMO: -5.96474 LUMO: 0.29660 factor:1 | 1 (-0.81966) | -1 | -1 |
| G: -5683.64846 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.93100 HOMO: -7.00421 LUMO: 0.08708 factor:1 | 1 (-1.91685) | -1 | -1 |
| G: -5683.64846 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.66144 HOMO: -5.40418 LUMO: 0.90070 factor:1 | -1 (0.35271) | -1 | -1 |
| G: -5683.64846 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.78097 HOMO: -7.00421 LUMO: -0.30477 factor:1 | 1 (-0.76682) | -1 | -1 |
| G: -5683.64846 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.39662 HOMO: -5.85861 LUMO: 0.74015 factor:1 | -1 (0.61754) | -1 | -1 |
| G: -5683.64846 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11946.73244 HOMO: -5.71439 LUMO: 0.26395 factor:1 | -1 (1.28171) | -1 | -1 |
| G: -5683.64846 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.27060 HOMO: -7.13755 LUMO: -0.78369 factor:1 | -1 (0.74355) | 1 | -1 |
| G: -5683.64846 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.05730 HOMO: -7.31442 LUMO: -0.98233 factor:1 | 1 (-1.04315) | 1 | -1 |
| G: -5683.64846 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.75702 HOMO: -7.25728 LUMO: -1.00410 factor:1 | 1 (-0.74287) | 1 | -1 |
| G: -5683.64846 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.52350 HOMO: -7.48585 LUMO: -0.83811 factor:1 | -1 (0.49065) | 1 | -1 |
| G: -5683.64846 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.01115 HOMO: -7.24911 LUMO: -0.77280 factor:1 | 1 (-0.99700) | 1 | -1 |
| G: -5683.64846 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.76933 HOMO: -7.55116 LUMO: -1.19730 factor:1 | -1 (0.24482) | 1 | -1 |
| G: -5683.64846 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.70220 HOMO: -5.76881 LUMO: 0.28028 factor:1 | -1 (0.31195) | -1 | -1 |
| G: -5683.64846 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.09129 HOMO: -5.77153 LUMO: -0.26939 factor:1 | 1 (-1.07714) | -1 | -1 |
| G: -5683.64846 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.67525 HOMO: -5.82868 LUMO: 0.36735 factor:1 | 1 (-0.66110) | -1 | -1 |
| G: -5683.64846 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.31190 HOMO: -5.83140 LUMO: -0.17960 factor:1 | 1 (-0.29775) | -1 | -1 |
| G: -5683.64846 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.75213 HOMO: -6.28855 LUMO: 0.01088 factor:1 | -1 (0.26202) | -1 | -1 |
| G: -5683.64846 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.32204 HOMO: -6.31576 LUMO: 0.25307 factor:1 | 1 (-1.30789) | -1 | -1 |
| G: -5683.64846 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.83626 HOMO: -7.06408 LUMO: -2.76196 factor:1 | 1 (-0.82211) | -1 | -1 |
| G: -5683.64846 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.22870 HOMO: -5.95657 LUMO: 0.37552 factor:1 | 1 (-1.21455) | -1 | -1 |
| G: -5683.64846 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.32468 HOMO: -6.61781 LUMO: 0.02721 factor:1 | 1 (-1.31053) | -1 | -1 |
| G: -5683.64846 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.51381 HOMO: -6.26678 LUMO: -0.66668 factor:1 | 1 (-0.49966) | -1 | -1 |
| G: -5683.64846 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.57844 HOMO: -6.00011 LUMO: -0.13334 factor:1 | -1 (0.43571) | -1 | -1 |
| G: -5683.64846 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.89068 HOMO: -5.60555 LUMO: 0.67484 factor:1 | 1 (-0.87653) | -1 | -1 |
| G: -5683.64846 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.96378 HOMO: -5.79875 LUMO: 0.99049 factor:1 | -1 (0.05037) | -1 | -1 |
| G: -5683.64846 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.96927 HOMO: -5.97834 LUMO: 0.48436 factor:1 | 1 (-0.95512) | -1 | -1 |
| G: -5683.64846 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.29021 HOMO: -5.82868 LUMO: 0.91974 factor:1 | 1 (-0.27606) | -1 | -1 |
| G: -5683.64846 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.90110 HOMO: -5.86677 LUMO: 0.99594 factor:1 | 1 (-1.88695) | -1 | -1 |
| G: -5683.64846 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.95536 HOMO: -5.70079 LUMO: 0.48980 factor:1 | 1 (-1.94121) | -1 | -1 |
| G: -5683.64846 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.01640 HOMO: -7.39605 LUMO: -1.02315 factor:1 | 1 (-1.00225) | 1 | -1 |
| G: -5683.64846 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.19124 HOMO: -7.22734 LUMO: -1.12927 factor:1 | 1 (-0.17709) | 1 | -1 |
| G: -5683.64846 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.63921 HOMO: -7.58926 LUMO: -0.65035 factor:1 | 1 (-2.62506) | 1 | 1 |
| G: -5683.64846 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.91082 HOMO: -7.43959 LUMO: -0.75648 factor:1 | 1 (-0.89667) | 1 | 1 |
| G: -5683.64846 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.52017 HOMO: -7.55388 LUMO: -1.15104 factor:1 | 1 (-1.50601) | 1 | -1 |
| G: -5683.64846 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.51327 HOMO: -6.74570 LUMO: -2.85447 factor:1 | 1 (-2.49912) | -1 | -1 |
| G: -5683.64846 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.35687 HOMO: -7.35524 LUMO: -1.25444 factor:1 | 1 (-1.34272) | 1 | 1 |
| G: -5683.64846 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.24523 HOMO: -6.81645 LUMO: -1.20819 factor:1 | 1 (-0.23108) | -1 | -1 |
| G: -5683.64846 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.78373 HOMO: -6.99605 LUMO: -1.62996 factor:1 | 1 (-2.76957) | -1 | -1 |
| G: -5683.64846 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.39252 HOMO: -6.88992 LUMO: -0.47620 factor:1 | 1 (-1.37837) | -1 | -1 |
| G: -5683.64846 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.55569 HOMO: -7.22190 LUMO: -0.01905 factor:1 | 1 (-0.54153) | 1 | 1 |
| G: -5683.64846 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.51708 HOMO: -6.77836 LUMO: -0.82995 factor:1 | -1 (0.49707) | -1 | -1 |
| G: -5683.64846 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.64830 HOMO: -6.48447 LUMO: -0.95512 factor:1 | 1 (-1.63415) | -1 | -1 |
| G: -5683.64846 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.40537 HOMO: -7.81239 LUMO: 1.22179 factor:1 | 1 (-0.39122) | 1 | 1 |
| G: -5683.64846 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.92288 HOMO: -7.36612 LUMO: 0.19320 factor:1 | -1 (0.09127) | 1 | 1 |
| G: -5683.64846 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.00627 HOMO: -7.24095 LUMO: 0.33470 factor:1 | 1 (-1.99212) | 1 | 1 |
| G: -5683.64846 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.83330 HOMO: -7.15932 LUMO: -2.24222 factor:1 | 1 (-0.81914) | -1 | -1 |
| G: -5683.64846 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.89127 HOMO: -6.88992 LUMO: -2.69937 factor:1 | 1 (-1.87712) | -1 | -1 |
| G: -5683.64846 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.86535 HOMO: -6.97428 LUMO: -0.98233 factor:1 | 1 (-0.85120) | -1 | -1 |
| G: -5683.64846 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.83022 HOMO: -7.17564 LUMO: -0.93879 factor:1 | 1 (-0.81607) | 1 | 1 |
| G: -5683.64846 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.61655 HOMO: -6.81645 LUMO: -1.14288 factor:1 | 1 (-1.60240) | -1 | -1 |
| G: -5683.64846 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.83025 HOMO: -6.83006 LUMO: -0.63403 factor:1 | 1 (-0.81610) | -1 | -1 |
| G: -5683.64846 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.70655 HOMO: -7.17292 LUMO: -1.07213 factor:1 | 1 (-0.69239) | 1 | 1 |
| G: -5683.64846 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.66550 HOMO: -7.53755 LUMO: 0.15510 factor:1 | 1 (-1.65135) | 1 | 1 |
| G: -5683.64846 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.94380 HOMO: -6.50080 LUMO: -0.51702 factor:1 | 1 (-0.92965) | -1 | -1 |
| G: -5683.64846 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.96013 HOMO: -6.72665 LUMO: -0.80001 factor:1 | 1 (-0.94598) | -1 | -1 |
| G: -5683.64846 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.38948 HOMO: -6.72665 LUMO: 1.68711 factor:1 | 1 (-0.37533) | -1 | -1 |
| G: -5683.64846 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.31576 HOMO: -7.11850 LUMO: -0.75103 factor:1 | 1 (-0.30161) | 1 | 1 |
| G: -5683.64846 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.54186 HOMO: -6.87087 LUMO: -0.85988 factor:1 | 1 (-0.52771) | -1 | -1 |
| G: -5683.64846 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.51598 HOMO: -7.08857 LUMO: -0.89798 factor:1 | 1 (-1.50182) | 1 | 1 |
| G: -5683.64846 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.57377 HOMO: -6.71305 LUMO: -0.85444 factor:1 | 1 (-1.55962) | -1 | -1 |
| G: -5683.64846 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.42800 HOMO: -6.59332 LUMO: -0.60137 factor:1 | 1 (-1.41385) | -1 | -1 |
| G: -5683.64846 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.29148 HOMO: -7.28993 LUMO: 0.03265 factor:1 | 1 (-1.27733) | 1 | 1 |
| G: -5683.64846 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.55421 HOMO: -7.32258 LUMO: 0.13878 factor:1 | 1 (-1.54006) | 1 | 1 |
| G: -5683.64846 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.74929 HOMO: -7.28993 LUMO: 0.11429 factor:1 | 1 (-1.73513) | 1 | 1 |
| G: -5683.64846 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.43671 HOMO: -6.86271 LUMO: -1.03947 factor:1 | 1 (-1.42256) | -1 | -1 |
| G: -5683.64846 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.62429 HOMO: -6.55794 LUMO: -0.84900 factor:1 | 1 (-0.61013) | -1 | -1 |
| G: -5683.64846 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.39774 HOMO: -7.03686 LUMO: 0.11429 factor:1 | 1 (-1.38359) | -1 | -1 |
| G: -5683.64846 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.56308 HOMO: -7.06952 LUMO: -0.96056 factor:1 | 1 (-1.54893) | 1 | 1 |
| G: -5683.64846 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.36936 HOMO: -6.90897 LUMO: -0.99866 factor:1 | 1 (-1.35521) | -1 | -1 |
| G: -5683.64846 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.53404 HOMO: -7.00693 LUMO: -0.83539 factor:1 | 1 (-1.51989) | -1 | -1 |
| G: -5683.64846 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.46967 HOMO: -6.74298 LUMO: -0.85172 factor:1 | 1 (-0.45552) | -1 | -1 |
| G: -5683.64846 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.09395 HOMO: -6.83822 LUMO: -1.07213 factor:1 | 1 (-2.07979) | -1 | -1 |
| G: -5683.64846 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.44969 HOMO: -7.21918 LUMO: -1.55377 factor:1 | 1 (-1.43554) | 1 | 1 |
| G: -5683.64846 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.31409 HOMO: -6.84094 LUMO: -1.09934 factor:1 | 1 (-1.29994) | -1 | -1 |
| G: -5683.64846 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.40121 HOMO: -7.09129 LUMO: -0.85988 factor:1 | 1 (-0.38705) | 1 | 1 |
| G: -5683.64846 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.42829 HOMO: -6.57971 LUMO: -2.27215 factor:1 | -1 (0.58586) | -1 | -1 |
| G: -5683.64846 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.53625 HOMO: -6.81373 LUMO: -1.86942 factor:1 | 1 (-1.52210) | -1 | -1 |
| G: -5683.64846 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.57269 HOMO: -6.59060 LUMO: -2.30480 factor:1 | 1 (-0.55854) | -1 | -1 |
| G: -5683.64846 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.72449 HOMO: -6.72938 LUMO: -1.23540 factor:1 | -1 (0.28967) | -1 | -1 |
| G: -5683.64846 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.76557 HOMO: -6.94707 LUMO: -2.62318 factor:1 | 1 (-0.75142) | -1 | -1 |
| G: -5683.64846 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.54075 HOMO: -7.28177 LUMO: -0.09796 factor:1 | 1 (-0.52659) | 1 | 1 |
| G: -5683.64846 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.69713 HOMO: -6.80013 LUMO: -0.79729 factor:1 | 1 (-0.68298) | -1 | -1 |
| G: -5683.64846 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.82829 HOMO: -7.26544 LUMO: 0.12789 factor:1 | 1 (-0.81414) | 1 | 1 |
| G: -5683.64846 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.50641 HOMO: -6.51713 LUMO: -0.49253 factor:1 | 1 (-0.49225) | -1 | -1 |
| G: -5683.64846 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.72870 HOMO: -6.68856 LUMO: -0.77280 factor:1 | 1 (-0.71454) | -1 | -1 |
| G: -5683.64846 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.77621 HOMO: -6.41100 LUMO: -0.70750 factor:1 | 1 (-0.76205) | -1 | -1 |
| G: -5683.64846 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.63721 HOMO: -7.56204 LUMO: 0.22041 factor:1 | 1 (-0.62306) | 1 | 1 |
| G: -5683.64846 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.58235 HOMO: -6.68312 LUMO: 1.30343 factor:1 | 1 (-0.56820) | -1 | -1 |
| G: -5683.64846 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.46621 HOMO: -7.24367 LUMO: 0.17415 factor:1 | 1 (-0.45206) | 1 | 1 |
| G: -5683.64846 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.74429 HOMO: -7.52395 LUMO: 1.16737 factor:1 | 1 (-0.73014) | 1 | 1 |
| G: -5683.64846 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.46806 HOMO: -6.89264 LUMO: 0.23130 factor:1 | 1 (-0.45391) | -1 | -1 |
| G: -5683.64846 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.37590 HOMO: -7.21102 LUMO: 0.19048 factor:1 | 1 (-0.36175) | 1 | 1 |
| G: -5683.64846 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.32861 HOMO: -7.08312 LUMO: 0.25034 factor:1 | 1 (-0.31445) | 1 | 1 |
| G: -5683.64846 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.66529 HOMO: -6.49536 LUMO: -0.65852 factor:1 | 1 (-0.65114) | -1 | -1 |
| G: -5683.64846 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.53079 HOMO: -6.85455 LUMO: 0.13606 factor:1 | 1 (-0.51664) | -1 | -1 |
| G: -5683.64846 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11946.93527 HOMO: -7.10217 LUMO: 0.35919 factor:1 | -1 (1.07888) | 1 | 1 |
| G: -5683.64846 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.25841 HOMO: -7.77429 LUMO: 1.19186 factor:1 | -1 (0.75574) | 1 | 1 |
| G: -5683.64846 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.96509 HOMO: -6.57427 LUMO: -0.50069 factor:1 | -1 (0.04906) | -1 | -1 |
| G: -5683.64846 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.87072 HOMO: -7.36340 LUMO: 0.10068 factor:1 | -1 (0.14343) | 1 | 1 |
| G: -5683.64846 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.47392 HOMO: -7.28177 LUMO: 0.15238 factor:1 | 1 (-0.45976) | 1 | 1 |
| G: -5683.64846 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.15021 HOMO: -6.86543 LUMO: -0.84355 factor:1 | 1 (-0.13606) | -1 | -1 |
| G: -5683.64846 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.19772 HOMO: -6.55794 LUMO: 1.39594 factor:1 | 1 (-0.18357) | -1 | -1 |
| G: -5683.64846 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.15149 HOMO: -6.26134 LUMO: 1.53744 factor:1 | 1 (-0.13734) | -1 | -1 |
| G: -5683.64846 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.70461 HOMO: -5.97562 LUMO: 1.42316 factor:1 | 1 (-0.69046) | -1 | -1 |
| G: -5683.64846 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.38063 HOMO: -6.65046 LUMO: 1.44492 factor:1 | 1 (-0.36648) | -1 | -1 |
| G: -5683.64846 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11945.63430 HOMO: -6.92258 LUMO: 0.17415 factor:1 | -1 (2.37985) | -1 | -1 |
| G: -5683.64846 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11945.65729 HOMO: -7.40966 LUMO: 0.19592 factor:1 | -1 (2.35686) | 1 | 1 |
| G: -5683.64846 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11945.84970 HOMO: -7.17564 LUMO: 0.16871 factor:1 | -1 (2.16445) | 1 | 1 |
| G: -5683.64846 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11945.88206 HOMO: -7.46953 LUMO: 0.22313 factor:1 | -1 (2.13209) | 1 | 1 |
| G: -5683.64846 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.47661 HOMO: -6.13345 LUMO: 1.85854 factor:1 | 1 (-0.46246) | -1 | -1 |
| G: -5683.64846 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.73925 HOMO: -6.99333 LUMO: -1.65717 factor:1 | 1 (-0.72510) | -1 | -1 |
| G: -5683.64846 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.66429 HOMO: -6.93074 LUMO: -1.79323 factor:1 | 1 (-0.65013) | -1 | -1 |
| G: -5683.64846 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.52175 HOMO: -6.87904 LUMO: -1.79323 factor:1 | 1 (-0.50760) | -1 | -1 |
| G: -5683.64846 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.88373 HOMO: -6.84094 LUMO: 0.66940 factor:1 | -1 (0.13042) | -1 | -1 |
| G: -5683.64846 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.45076 HOMO: -7.13210 LUMO: -1.17553 factor:1 | 1 (-0.43661) | 1 | 1 |
| G: -5683.64846 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.78726 HOMO: -6.52801 LUMO: -2.23678 factor:1 | -1 (0.22689) | -1 | -1 |
| G: -5683.64846 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.85883 HOMO: -6.81917 LUMO: -1.86398 factor:1 | -1 (0.15532) | -1 | -1 |
| G: -5683.64846 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.80098 HOMO: -7.30626 LUMO: -1.66806 factor:1 | -1 (0.21317) | 1 | 1 |
| G: -5683.64846 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.69324 HOMO: -6.98516 LUMO: -1.40683 factor:1 | 1 (-0.67909) | -1 | -1 |
| G: -5683.64846 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.06406 HOMO: -6.95523 LUMO: -0.97145 factor:1 | 1 (-0.04991) | -1 | -1 |
| G: -5683.64846 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.12536 HOMO: -6.83278 LUMO: -2.68848 factor:1 | 1 (-0.11121) | -1 | -1 |
| G: -5683.64846 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.07347 HOMO: -7.25456 LUMO: -2.97420 factor:1 | 1 (-0.05932) | -1 | -1 |
| G: -5683.64846 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.44534 HOMO: -6.80557 LUMO: -2.65039 factor:1 | 1 (-0.43119) | -1 | -1 |
| G: -5683.64846 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.71642 HOMO: -7.10489 LUMO: 0.77008 factor:1 | 1 (-0.70227) | 1 | -1 |
| G: -5683.64846 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11945.30692 HOMO: -7.28993 LUMO: -1.06124 factor:1 | -1 (2.70723) | 1 | 1 |
| G: -5683.64846 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11945.29622 HOMO: -7.11578 LUMO: -1.10206 factor:1 | -1 (2.71793) | 1 | 1 |
| G: -5683.64846 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11945.52594 HOMO: -6.91713 LUMO: -1.36329 factor:1 | -1 (2.48821) | -1 | -1 |
| G: -5683.64846 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11945.60254 HOMO: -7.07224 LUMO: 0.51974 factor:1 | -1 (2.41161) | 1 | 1 |
| G: -5683.64846 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.62168 HOMO: -7.22734 LUMO: -0.93335 factor:1 | 1 (-2.60753) | 1 | 1 |
| G: -5683.64846 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.92347 HOMO: -7.19469 LUMO: -0.96600 factor:1 | 1 (-1.90931) | 1 | 1 |
| G: -5683.64846 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.34721 HOMO: -6.93890 LUMO: -0.66940 factor:1 | 1 (-1.33306) | -1 | -1 |
| G: -5683.64846 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.05977 HOMO: -7.09673 LUMO: -1.05852 factor:1 | 1 (-2.04562) | 1 | 1 |
| G: -5683.64846 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.10750 HOMO: -7.19197 LUMO: -2.26943 factor:1 | 1 (-2.09334) | -1 | -1 |
| G: -5683.64846 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.60841 HOMO: -6.90081 LUMO: -2.64767 factor:1 | 1 (-1.59426) | -1 | -1 |
| G: -5683.64846 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.30372 HOMO: -6.93890 LUMO: -2.65039 factor:1 | 1 (-2.28957) | -1 | -1 |
| G: -5683.64846 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.49990 HOMO: -6.80013 LUMO: -2.54154 factor:1 | 1 (-0.48575) | -1 | -1 |
| G: -5683.64846 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.87501 HOMO: -6.68040 LUMO: -0.89798 factor:1 | 1 (-0.86086) | -1 | -1 |
| G: -5683.64846 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.88618 HOMO: -7.01782 LUMO: -1.09662 factor:1 | 1 (-2.87203) | -1 | -1 |
| G: -5683.64846 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.22603 HOMO: -6.58516 LUMO: -0.83539 factor:1 | 1 (-2.21188) | -1 | -1 |
| G: -5683.64846 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.04826 HOMO: -7.46953 LUMO: 0.06259 factor:1 | 1 (-2.03411) | 1 | 1 |
| G: -5683.64846 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.99767 HOMO: -6.96884 LUMO: -0.99866 factor:1 | 1 (-1.98352) | -1 | -1 |
| G: -5683.64846 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.29591 HOMO: -7.29809 LUMO: -0.19320 factor:1 | 1 (-2.28176) | 1 | 1 |
| G: -5683.64846 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.22448 HOMO: -6.86271 LUMO: 0.04082 factor:1 | 1 (-2.21033) | -1 | -1 |
| G: -5683.64846 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.81972 HOMO: -6.36746 LUMO: -1.02587 factor:1 | 1 (-0.80557) | -1 | -1 |
| G: -5683.64846 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.13060 HOMO: -7.15659 LUMO: -1.25989 factor:1 | 1 (-2.11645) | 1 | 1 |
| G: -5683.64846 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.10712 HOMO: -6.69128 LUMO: -0.59865 factor:1 | 1 (-2.09296) | -1 | -1 |
| G: -5683.64846 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.41263 HOMO: -7.09129 LUMO: -1.08573 factor:1 | 1 (-1.39847) | 1 | 1 |
| G: -5683.64846 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.35920 HOMO: -6.64502 LUMO: -0.66396 factor:1 | 1 (-2.34505) | -1 | -1 |
| G: -5683.64846 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.66107 HOMO: -6.93346 LUMO: -0.87349 factor:1 | 1 (-1.64691) | -1 | -1 |
| G: -5683.64846 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.61201 HOMO: -6.77019 LUMO: -0.87349 factor:1 | 1 (-0.59786) | -1 | -1 |
| G: -5683.64846 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.54009 HOMO: -6.59060 LUMO: -0.82995 factor:1 | 1 (-0.52594) | -1 | -1 |
| G: -5683.64846 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.77550 HOMO: -7.17564 LUMO: -1.08846 factor:1 | 1 (-0.76135) | 1 | 1 |
| G: -5683.64846 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11945.21622 HOMO: -7.27088 LUMO: -1.18642 factor:1 | -1 (2.79793) | 1 | 1 |
| G: -5683.64846 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11945.73982 HOMO: -7.06680 LUMO: -1.13199 factor:1 | -1 (2.27433) | 1 | 1 |
| G: -5683.64846 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.50594 HOMO: -7.21918 LUMO: -1.03947 factor:1 | 1 (-0.49179) | 1 | 1 |
| G: -5683.64846 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.85042 HOMO: -7.26000 LUMO: -0.11973 factor:1 | -1 (0.16373) | 1 | 1 |
| G: -5683.64846 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.00378 HOMO: -6.77564 LUMO: 0.23402 factor:1 | -1 (0.01037) | -1 | -1 |
| G: -5683.64846 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.65991 HOMO: -7.07224 LUMO: -0.75648 factor:1 | -1 (0.35424) | 1 | 1 |
| G: -5683.64846 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.36197 HOMO: -7.45048 LUMO: 0.18232 factor:1 | 1 (-0.34782) | 1 | 1 |
| G: -5683.64846 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.72125 HOMO: -7.48313 LUMO: 0.15238 factor:1 | -1 (0.29290) | 1 | 1 |
| G: -5683.64846 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.26950 HOMO: -6.60692 LUMO: -0.50885 factor:1 | 1 (-0.25535) | -1 | -1 |
| G: -5683.64846 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.88969 HOMO: -6.62869 LUMO: -0.60954 factor:1 | -1 (0.12446) | -1 | -1 |
| G: -5683.64846 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.62888 HOMO: -7.40422 LUMO: -1.28982 factor:1 | 1 (-0.61473) | 1 | 1 |
| G: -5683.64846 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.95807 HOMO: -6.75114 LUMO: -1.23268 factor:1 | -1 (0.05608) | -1 | -1 |
| G: -5683.64846 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.89137 HOMO: -6.84638 LUMO: -0.73199 factor:1 | -1 (0.12278) | -1 | -1 |
| G: -5683.64846 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.07095 HOMO: -6.79196 LUMO: -1.43676 factor:1 | -1 (0.94320) | -1 | -1 |
| G: -5683.64846 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11946.97353 HOMO: -7.00965 LUMO: -1.37690 factor:1 | -1 (1.04062) | -1 | -1 |
| G: -5683.64846 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.16880 HOMO: -6.97972 LUMO: -1.58098 factor:1 | -1 (0.84535) | -1 | -1 |
| G: -5683.64846 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.11609 HOMO: -6.91169 LUMO: -1.48574 factor:1 | -1 (0.89806) | -1 | -1 |
| G: -5683.64846 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.16482 HOMO: -6.90081 LUMO: -1.30343 factor:1 | 1 (-0.15067) | -1 | -1 |
| G: -5683.64846 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.73738 HOMO: -6.78652 LUMO: -1.51840 factor:1 | -1 (0.27677) | -1 | -1 |
| G: -5683.64846 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.01769 HOMO: -6.84638 LUMO: -1.15104 factor:1 | 1 (-0.00354) | -1 | -1 |
| G: -5683.64846 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.69412 HOMO: -6.61237 LUMO: -0.89798 factor:1 | -1 (0.32003) | -1 | -1 |
| G: -5683.64846 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.64968 HOMO: -7.16204 LUMO: -1.30070 factor:1 | -1 (0.36447) | 1 | 1 |
| G: -5683.64846 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.23750 HOMO: -7.32803 LUMO: 0.14694 factor:1 | 1 (-0.22335) | 1 | 1 |
| G: -5683.64846 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.89401 HOMO: -6.99877 LUMO: -0.87621 factor:1 | -1 (0.12014) | -1 | -1 |
| G: -5683.64846 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.94944 HOMO: -6.99877 LUMO: -0.97145 factor:1 | -1 (0.06471) | -1 | -1 |
| G: -5683.64846 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.68638 HOMO: -7.08040 LUMO: -1.09662 factor:1 | 1 (-0.67223) | 1 | 1 |
| G: -5683.64846 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.47275 HOMO: -6.90897 LUMO: -1.14016 factor:1 | 1 (-0.45859) | -1 | -1 |
| G: -5683.64846 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.32961 HOMO: -6.68312 LUMO: -0.74831 factor:1 | 1 (-0.31546) | -1 | -1 |
| G: -5683.64846 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.55716 HOMO: -6.99061 LUMO: -0.86804 factor:1 | 1 (-0.54300) | -1 | -1 |
| G: -5683.64846 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.59521 HOMO: -7.10761 LUMO: -1.18642 factor:1 | 1 (-2.58105) | 1 | 1 |
| G: -5683.64846 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.83560 HOMO: -6.79196 LUMO: -0.71294 factor:1 | 1 (-1.82145) | -1 | -1 |
| G: -5683.64846 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.89949 HOMO: -6.86271 LUMO: -0.81362 factor:1 | 1 (-1.88534) | -1 | -1 |
| G: -5683.64846 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.06894 HOMO: -7.01510 LUMO: -0.99322 factor:1 | 1 (-2.05479) | -1 | -1 |
| G: -5683.64846 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.13811 HOMO: -6.88720 LUMO: -0.87893 factor:1 | 1 (-2.12396) | -1 | -1 |
| G: -5683.64846 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.65519 HOMO: -6.88448 LUMO: 0.22041 factor:1 | 1 (-1.64104) | -1 | -1 |
| G: -5683.64846 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.98837 HOMO: -7.55932 LUMO: 1.12111 factor:1 | 1 (-1.97421) | 1 | 1 |
| G: -5683.64846 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.99773 HOMO: -6.46815 LUMO: -0.86260 factor:1 | 1 (-1.98357) | -1 | -1 |
| G: -5683.64846 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.29502 HOMO: -7.13755 LUMO: 0.23130 factor:1 | 1 (-1.28087) | 1 | 1 |
| G: -5683.64846 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.42027 HOMO: -6.78924 LUMO: 1.51023 factor:1 | 1 (-1.40612) | -1 | -1 |
| G: -5683.64846 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.14491 HOMO: -6.48992 LUMO: 1.74969 factor:1 | 1 (-2.13076) | -1 | -1 |
| G: -5683.64846 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.46310 HOMO: -6.78380 LUMO: 1.81500 factor:1 | 1 (-1.44895) | -1 | -1 |
| G: -5683.64846 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.44025 HOMO: -6.49536 LUMO: 1.70615 factor:1 | 1 (-0.42610) | -1 | -1 |
| G: -5683.64846 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.68951 HOMO: -6.38651 LUMO: 1.44492 factor:1 | 1 (-0.67536) | -1 | -1 |
| G: -5683.64846 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.77436 HOMO: -6.83822 LUMO: 1.38234 factor:1 | 1 (-0.76020) | -1 | -1 |
| G: -5683.64846 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.60252 HOMO: -6.01644 LUMO: 1.20274 factor:1 | 1 (-0.58836) | -1 | -1 |
| G: -5683.64846 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.47906 HOMO: -6.18243 LUMO: 1.77962 factor:1 | 1 (-0.46491) | -1 | -1 |
| G: -5683.64846 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.48815 HOMO: -6.81917 LUMO: -1.01771 factor:1 | 1 (-0.47400) | -1 | -1 |
| G: -5683.64846 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.70943 HOMO: -6.61237 LUMO: -0.91702 factor:1 | 1 (-0.69528) | -1 | -1 |
| G: -5683.64846 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.40991 HOMO: -6.84094 LUMO: -0.84900 factor:1 | 1 (-0.39576) | -1 | -1 |
| G: -5683.64846 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.68807 HOMO: -6.81917 LUMO: -1.01771 factor:1 | 1 (-0.67392) | -1 | -1 |
| G: -5683.64846 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.16197 HOMO: -7.86953 LUMO: 1.16737 factor:1 | 1 (-2.14782) | 1 | 1 |
| G: -5683.64846 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.52129 HOMO: -7.40694 LUMO: 0.11429 factor:1 | 1 (-0.50714) | 1 | 1 |
| G: -5683.64846 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.33038 HOMO: -6.70489 LUMO: -0.65035 factor:1 | 1 (-0.31622) | -1 | -1 |
| G: -5683.64846 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.45174 HOMO: -7.23279 LUMO: 0.33470 factor:1 | 1 (-0.43759) | 1 | 1 |
| G: -5683.64846 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.50583 HOMO: -7.17020 LUMO: 0.41361 factor:1 | 1 (-0.49168) | 1 | 1 |
| G: -5683.64846 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.68940 HOMO: -6.90353 LUMO: -0.90070 factor:1 | 1 (-0.67525) | -1 | -1 |
| G: -5683.64846 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.56195 HOMO: -7.39061 LUMO: 0.17687 factor:1 | -1 (0.45220) | 1 | 1 |
| G: -5683.64846 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.89320 HOMO: -7.16748 LUMO: 0.42178 factor:1 | -1 (0.12095) | 1 | 1 |
| G: -5683.64846 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.45244 HOMO: -7.36884 LUMO: -1.11295 factor:1 | 1 (-1.43829) | 1 | 1 |
| G: -5683.64846 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.65134 HOMO: -7.33347 LUMO: 0.33198 factor:1 | -1 (0.36281) | 1 | 1 |
| G: -5683.64846 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.87357 HOMO: -7.31986 LUMO: -0.83539 factor:1 | 1 (-0.85942) | 1 | 1 |
| G: -5683.64846 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.93790 HOMO: -7.31170 LUMO: 0.08708 factor:1 | 1 (-0.92374) | 1 | 1 |
| G: -5683.64846 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.83237 HOMO: -7.36884 LUMO: 0.38096 factor:1 | 1 (-0.81822) | 1 | 1 |
| G: -5683.64846 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.01662 HOMO: -6.99333 LUMO: 1.74153 factor:1 | 1 (-1.00247) | -1 | -1 |
| G: -5683.64846 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.19265 HOMO: -6.94435 LUMO: 1.74969 factor:1 | 1 (-1.17850) | -1 | -1 |
| G: -5683.64846 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.12125 HOMO: -7.02598 LUMO: 1.43404 factor:1 | 1 (-1.10710) | -1 | -1 |
| G: -5683.64846 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.24405 HOMO: -6.41100 LUMO: 1.62996 factor:1 | 1 (-1.22990) | -1 | -1 |
| G: -5683.64846 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.59483 HOMO: -6.57699 LUMO: 1.81228 factor:1 | 1 (-2.58067) | -1 | -1 |
| G: -5683.64846 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.58248 HOMO: -6.86543 LUMO: 1.49935 factor:1 | 1 (-1.56833) | -1 | -1 |
| G: -5683.64846 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.64501 HOMO: -6.91169 LUMO: -1.22451 factor:1 | 1 (-1.63086) | -1 | -1 |
| G: -5683.64846 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.84616 HOMO: -7.09945 LUMO: -1.23812 factor:1 | 1 (-1.83201) | 1 | 1 |
| G: -5683.64846 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.98016 HOMO: -7.48857 LUMO: 0.10340 factor:1 | 1 (-0.96600) | 1 | 1 |
| G: -5683.64846 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.29877 HOMO: -7.21918 LUMO: -0.06803 factor:1 | 1 (-1.28462) | 1 | 1 |
| G: -5683.64846 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.44016 HOMO: -6.34025 LUMO: -0.68845 factor:1 | 1 (-1.42601) | -1 | -1 |
| G: -5683.64846 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.29208 HOMO: -6.82734 LUMO: -0.77825 factor:1 | 1 (-1.27793) | -1 | -1 |
| G: -5683.64846 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.52735 HOMO: -6.92258 LUMO: -1.03675 factor:1 | 1 (-1.51320) | -1 | -1 |
| G: -5683.64846 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.62778 HOMO: -6.42461 LUMO: -0.95240 factor:1 | -1 (0.38637) | -1 | -1 |
| G: -5683.64846 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.44175 HOMO: -6.96067 LUMO: -1.05036 factor:1 | 1 (-0.42760) | -1 | -1 |
| G: -5683.64846 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.37658 HOMO: -7.23551 LUMO: 0.12245 factor:1 | 1 (-0.36243) | 1 | 1 |
| G: -5683.64846 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.57732 HOMO: -6.85183 LUMO: 0.16055 factor:1 | 1 (-0.56317) | -1 | -1 |
| G: -5683.64846 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.56472 HOMO: -6.46815 LUMO: -0.89253 factor:1 | 1 (-0.55057) | -1 | -1 |
| G: -5683.64846 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.46175 HOMO: -7.23823 LUMO: -0.06259 factor:1 | 1 (-0.44760) | 1 | 1 |
| G: -5683.64846 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.38099 HOMO: -6.76475 LUMO: -0.99049 factor:1 | 1 (-0.36684) | -1 | -1 |
| G: -5683.64846 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.59833 HOMO: -7.14843 LUMO: -0.88165 factor:1 | 1 (-0.58417) | 1 | 1 |
| G: -5683.64846 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.57101 HOMO: -7.15659 LUMO: 0.20681 factor:1 | 1 (-0.55685) | 1 | 1 |
| G: -5683.64846 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.67942 HOMO: -7.11306 LUMO: 0.14150 factor:1 | -1 (0.33473) | 1 | 1 |
| G: -5683.64846 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.23457 HOMO: -6.67223 LUMO: -0.86260 factor:1 | 1 (-2.22042) | -1 | -1 |
| G: -5683.64846 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.35159 HOMO: -6.92530 LUMO: 0.30749 factor:1 | 1 (-1.33744) | -1 | -1 |
| G: -5683.64846 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.52490 HOMO: -6.50624 LUMO: -0.70477 factor:1 | 1 (-1.51075) | -1 | -1 |
| G: -5683.64846 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.38952 HOMO: -7.35524 LUMO: 0.75103 factor:1 | 1 (-1.37537) | 1 | 1 |
| G: -5683.64846 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.59653 HOMO: -7.07768 LUMO: -0.26939 factor:1 | 1 (-0.58238) | 1 | 1 |
| G: -5683.64846 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.80764 HOMO: -7.15932 LUMO: 0.42450 factor:1 | -1 (0.20651) | 1 | 1 |
| G: -5683.64846 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.60169 HOMO: -7.46136 LUMO: 0.04626 factor:1 | 1 (-1.58754) | 1 | 1 |
| G: -5683.64846 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.72938 HOMO: -7.05047 LUMO: -1.06669 factor:1 | 1 (-0.71522) | -1 | -1 |
| G: -5683.64846 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.02697 HOMO: -6.66951 LUMO: -0.99322 factor:1 | 1 (-0.01282) | -1 | -1 |
| G: -5683.64846 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.94425 HOMO: -7.01782 LUMO: -1.08846 factor:1 | -1 (0.06991) | -1 | -1 |
| G: -5683.64846 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.08982 HOMO: -7.03959 LUMO: -1.15376 factor:1 | 1 (-1.07567) | -1 | -1 |
| G: -5683.64846 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.97278 HOMO: -6.68856 LUMO: 1.61364 factor:1 | 1 (-0.95863) | -1 | -1 |
| G: -5683.64846 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.07118 HOMO: -6.53345 LUMO: 1.60275 factor:1 | 1 (-1.05703) | -1 | -1 |
| G: -5683.64846 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.37586 HOMO: -6.73482 LUMO: 1.86398 factor:1 | 1 (-1.36171) | -1 | -1 |
| G: -5683.64846 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.21782 HOMO: -6.87632 LUMO: 1.59731 factor:1 | 1 (-1.20367) | -1 | -1 |
| G: -5683.64846 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.05727 HOMO: -6.31848 LUMO: 2.12521 factor:1 | 1 (-1.04312) | -1 | -1 |
| G: -5683.64846 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.69533 HOMO: -6.35114 LUMO: 1.71432 factor:1 | 1 (-0.68118) | -1 | -1 |
| G: -5683.64846 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.03161 HOMO: -6.34842 LUMO: 1.92929 factor:1 | 1 (-1.01746) | -1 | -1 |
| G: -5683.64846 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.92181 HOMO: -6.14977 LUMO: 1.78235 factor:1 | 1 (-0.90766) | -1 | -1 |
| G: -5683.64846 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.76940 HOMO: -6.31032 LUMO: 1.51567 factor:1 | 1 (-0.75525) | -1 | -1 |
| G: -5683.64846 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.88562 HOMO: -6.25862 LUMO: 1.75241 factor:1 | 1 (-0.87147) | -1 | -1 |
| G: -5683.64846 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.13153 HOMO: -6.49264 LUMO: 1.66806 factor:1 | 1 (-1.11738) | -1 | -1 |
| G: -5683.64846 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.13964 HOMO: -6.28311 LUMO: 1.60003 factor:1 | 1 (-1.12549) | -1 | -1 |
| G: -5683.64846 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.24465 HOMO: -7.13210 LUMO: -0.04354 factor:1 | 1 (-1.23050) | 1 | 1 |
| G: -5683.64846 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.06876 HOMO: -7.35252 LUMO: 0.03537 factor:1 | 1 (-1.05460) | 1 | 1 |
| G: -5683.64846 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.29284 HOMO: -6.58243 LUMO: -0.48980 factor:1 | 1 (-1.27869) | -1 | -1 |
| G: -5683.64846 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.11741 HOMO: -6.90081 LUMO: -0.05442 factor:1 | 1 (-1.10326) | -1 | -1 |
| G: -5683.64846 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.06960 HOMO: -7.22734 LUMO: 0.17143 factor:1 | 1 (-1.05545) | 1 | 1 |
| G: -5683.64846 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.94304 HOMO: -7.13210 LUMO: -0.99866 factor:1 | 1 (-0.92889) | 1 | 1 |
| G: -5683.64846 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.02663 HOMO: -7.39878 LUMO: 0.13334 factor:1 | 1 (-1.01248) | 1 | 1 |
| G: -5683.64846 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.28803 HOMO: -7.04503 LUMO: -0.89798 factor:1 | 1 (-1.27387) | -1 | -1 |
| G: -5683.64846 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.06631 HOMO: -6.95523 LUMO: -1.07213 factor:1 | 1 (-1.05216) | -1 | -1 |
| G: -5683.64846 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.05899 HOMO: -6.75114 LUMO: -1.28438 factor:1 | 1 (-1.04484) | -1 | -1 |
| G: -5683.64846 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.16849 HOMO: -6.75114 LUMO: -0.11701 factor:1 | 1 (-1.15433) | -1 | -1 |
| G: -5683.64846 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.02489 HOMO: -6.83278 LUMO: -0.01633 factor:1 | 1 (-1.01074) | -1 | -1 |
| G: -5683.64846 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.28789 HOMO: -6.93890 LUMO: -0.88981 factor:1 | 1 (-1.27374) | -1 | -1 |
| G: -5683.64846 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.16824 HOMO: -7.07224 LUMO: -1.08573 factor:1 | 1 (-1.15409) | 1 | 1 |
| G: -5683.64846 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.23679 HOMO: -6.99877 LUMO: -0.95240 factor:1 | 1 (-1.22263) | -1 | -1 |
| G: -5683.64846 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.01618 HOMO: -7.09129 LUMO: 0.35375 factor:1 | 1 (-1.00203) | 1 | 1 |
| G: -5683.64846 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.98818 HOMO: -7.09401 LUMO: 0.04354 factor:1 | 1 (-0.97403) | 1 | 1 |
| G: -5683.64846 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.86203 HOMO: -6.85183 LUMO: -0.68573 factor:1 | 1 (-0.84788) | -1 | -1 |
| G: -5683.64846 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.97901 HOMO: -6.83006 LUMO: -0.58777 factor:1 | 1 (-0.96486) | -1 | -1 |
| G: -5683.64846 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.53891 HOMO: -7.40422 LUMO: 0.17687 factor:1 | 1 (-1.52476) | 1 | 1 |
| G: -5683.64846 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.52702 HOMO: -7.15932 LUMO: 0.10340 factor:1 | 1 (-1.51287) | 1 | 1 |
| G: -5683.64846 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.98315 HOMO: -7.03414 LUMO: -0.19592 factor:1 | 1 (-0.96900) | -1 | -1 |
| G: -5683.64846 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.95967 HOMO: -6.48447 LUMO: -0.36191 factor:1 | 1 (-0.94551) | -1 | -1 |
| G: -5683.64846 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.71604 HOMO: -7.49402 LUMO: 0.11429 factor:1 | 1 (-0.70189) | 1 | 1 |
| G: -5683.64846 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.91588 HOMO: -7.01237 LUMO: -1.06397 factor:1 | 1 (-0.90173) | -1 | -1 |
| G: -5683.64846 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.06457 HOMO: -6.67223 LUMO: -1.07213 factor:1 | 1 (-1.05041) | -1 | -1 |
| G: -5683.64846 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.07999 HOMO: -7.38789 LUMO: -1.15376 factor:1 | 1 (-1.06584) | 1 | 1 |
| G: -5683.64846 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.96582 HOMO: -6.42461 LUMO: -1.23812 factor:1 | 1 (-0.95166) | -1 | -1 |
| G: -5683.64846 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.93237 HOMO: -7.36884 LUMO: -1.19186 factor:1 | 1 (-0.91822) | 1 | 1 |
| G: -5683.64846 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.07570 HOMO: -6.65591 LUMO: 0.07075 factor:1 | 1 (-1.06154) | -1 | -1 |
| G: -5683.64846 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.02995 HOMO: -7.39061 LUMO: -0.16871 factor:1 | 1 (-1.01580) | 1 | 1 |
| G: -5683.64846 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.92247 HOMO: -6.90353 LUMO: -0.96056 factor:1 | 1 (-0.90832) | -1 | -1 |
| G: -5683.64846 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.71199 HOMO: -7.42054 LUMO: 0.19048 factor:1 | 1 (-0.69784) | 1 | 1 |
| G: -5683.64846 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.37567 HOMO: -7.40150 LUMO: 0.35647 factor:1 | 1 (-1.36152) | 1 | 1 |
| G: -5683.64846 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.22985 HOMO: -6.56067 LUMO: -0.96056 factor:1 | 1 (-1.21570) | -1 | -1 |
| G: -5683.64846 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.93493 HOMO: -6.89809 LUMO: -0.81090 factor:1 | 1 (-0.92078) | -1 | -1 |
| G: -5683.64846 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.60663 HOMO: -6.91986 LUMO: -0.84900 factor:1 | 1 (-0.59247) | -1 | -1 |
| G: -5683.64846 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.92127 HOMO: -6.61509 LUMO: -0.62042 factor:1 | 1 (-0.90712) | -1 | -1 |
| G: -5683.64846 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.10114 HOMO: -6.58243 LUMO: -0.65579 factor:1 | 1 (-1.08699) | -1 | -1 |
| G: -5683.64846 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.89792 HOMO: -6.52257 LUMO: -0.92519 factor:1 | 1 (-0.88377) | -1 | -1 |
| G: -5683.64846 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.21115 HOMO: -6.69128 LUMO: 1.49118 factor:1 | 1 (-1.19700) | -1 | -1 |
| G: -5683.64846 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.89836 HOMO: -7.02870 LUMO: 1.67894 factor:1 | 1 (-0.88421) | -1 | -1 |
| G: -5683.64846 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.25096 HOMO: -6.88720 LUMO: 1.68711 factor:1 | 1 (-1.23681) | -1 | -1 |
| G: -5683.64846 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.11180 HOMO: -5.89943 LUMO: 1.03675 factor:1 | 1 (-1.09765) | -1 | -1 |
| G: -5683.64846 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.75757 HOMO: -6.40556 LUMO: 1.14560 factor:1 | 1 (-0.74342) | -1 | -1 |
| G: -5683.64846 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.65786 HOMO: -6.51168 LUMO: 1.48030 factor:1 | 1 (-0.64371) | -1 | -1 |
| G: -5683.64846 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.71838 HOMO: -6.64502 LUMO: 1.91568 factor:1 | 1 (-0.70423) | -1 | -1 |
| G: -5683.64846 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.63079 HOMO: -6.47903 LUMO: 1.91296 factor:1 | 1 (-0.61664) | -1 | -1 |
| G: -5683.64846 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.58369 HOMO: -6.34297 LUMO: 1.91840 factor:1 | 1 (-0.56953) | -1 | -1 |
| G: -5683.64846 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.67395 HOMO: -6.89809 LUMO: 1.82861 factor:1 | 1 (-0.65979) | -1 | -1 |
| G: -5683.64846 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.20397 HOMO: -6.10079 LUMO: 1.62996 factor:1 | 1 (-1.18982) | -1 | -1 |
| G: -5683.64846 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.96911 HOMO: -7.16476 LUMO: -0.92247 factor:1 | 1 (-0.95496) | 1 | 1 |
| G: -5683.64846 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.27505 HOMO: -7.10489 LUMO: -0.95784 factor:1 | 1 (-1.26089) | 1 | 1 |
| G: -5683.64846 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.72565 HOMO: -6.76475 LUMO: -0.99866 factor:1 | 1 (-0.71150) | -1 | -1 |
| G: -5683.64846 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.81057 HOMO: -6.81373 LUMO: -1.05036 factor:1 | 1 (-0.79642) | -1 | -1 |
| G: -5683.64846 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.85398 HOMO: -6.90081 LUMO: -1.03947 factor:1 | 1 (-0.83983) | -1 | -1 |
| G: -5683.64846 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.76200 HOMO: -7.06952 LUMO: -0.91702 factor:1 | 1 (-0.74785) | 1 | 1 |
| G: -5683.64846 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.87942 HOMO: -6.73482 LUMO: -0.94151 factor:1 | 1 (-0.86527) | -1 | -1 |
| G: -5683.64846 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.73114 HOMO: -6.99605 LUMO: -1.04764 factor:1 | 1 (-0.71699) | -1 | -1 |
| G: -5683.64846 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.70750 HOMO: -7.03686 LUMO: -0.93335 factor:1 | 1 (-0.69335) | -1 | -1 |
| G: -5683.64846 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.56423 HOMO: -6.81101 LUMO: -0.95240 factor:1 | 1 (-0.55008) | -1 | -1 |
| G: -5683.64846 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.64812 HOMO: -6.83822 LUMO: -0.65307 factor:1 | 1 (-0.63397) | -1 | -1 |
| G: -5683.64846 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.89648 HOMO: -7.05319 LUMO: -0.81634 factor:1 | 1 (-0.88233) | -1 | -1 |
| G: -5683.64846 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.74589 HOMO: -7.57565 LUMO: 0.19048 factor:1 | 1 (-0.73174) | 1 | 1 |
| G: -5683.64846 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.84851 HOMO: -6.56067 LUMO: -0.50613 factor:1 | 1 (-0.83436) | -1 | -1 |
| G: -5684.20830 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11946.80934 HOMO: -6.74298 LUMO: -0.70477 factor:1 | -1 (1.76466) | -1 | -1 |
| G: -5684.20830 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.33558 HOMO: -7.02054 LUMO: 0.03537 factor:1 | -1 (1.23842) | -1 | -1 |
| G: -5684.20830 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.38711 HOMO: -7.33347 LUMO: -0.17960 factor:1 | -1 (0.18689) | 1 | 1 |
| G: -5684.20830 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.11190 HOMO: -6.98244 LUMO: -0.88165 factor:1 | -1 (1.46209) | -1 | -1 |
| G: -5684.20830 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11946.98311 HOMO: -7.14843 LUMO: -1.19730 factor:1 | -1 (1.59089) | 1 | 1 |
| G: -5684.20830 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.98321 HOMO: -7.17564 LUMO: -1.21907 factor:1 | -1 (0.59079) | 1 | 1 |
| G: -5684.20830 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11946.64501 HOMO: -6.74026 LUMO: -0.86532 factor:1 | -1 (1.92899) | -1 | -1 |
| G: -5684.20830 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.15272 HOMO: -6.82462 LUMO: -1.24084 factor:1 | -1 (1.42128) | -1 | -1 |
| G: -5684.20830 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.29212 HOMO: -6.78924 LUMO: -0.70477 factor:1 | -1 (1.28187) | -1 | -1 |
| G: -5684.20830 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11946.89432 HOMO: -7.41238 LUMO: 0.05987 factor:1 | -1 (1.67968) | 1 | 1 |
| G: -5684.20830 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.17222 HOMO: -6.75931 LUMO: 0.02721 factor:1 | -1 (0.40178) | -1 | -1 |
| G: -5684.20830 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.44943 HOMO: -6.28583 LUMO: -0.93063 factor:1 | -1 (0.12457) | -1 | -1 |
| G: -5684.20830 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.26383 HOMO: -6.69128 LUMO: -0.83539 factor:1 | -1 (1.31017) | -1 | -1 |
| G: -5684.20830 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11946.91753 HOMO: -7.22190 LUMO: 0.01361 factor:1 | -1 (1.65647) | 1 | 1 |
| G: -5684.20830 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11946.87067 HOMO: -6.95251 LUMO: -1.09934 factor:1 | -1 (1.70332) | -1 | -1 |
| G: -5684.20830 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.35762 HOMO: -6.75387 LUMO: -0.90614 factor:1 | -1 (1.21638) | -1 | -1 |
| G: -5684.20830 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.02564 HOMO: -7.48585 LUMO: 0.05987 factor:1 | -1 (1.54836) | 1 | 1 |
| G: -5684.20830 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.23660 HOMO: -6.92802 LUMO: -0.66940 factor:1 | -1 (0.33739) | -1 | -1 |
| G: -5684.20830 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.33582 HOMO: -7.29537 LUMO: -0.14150 factor:1 | -1 (0.23818) | 1 | 1 |
| G: -5684.20830 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11946.95141 HOMO: -6.57155 LUMO: -0.86804 factor:1 | -1 (1.62259) | -1 | -1 |
| G: -5684.20830 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.02889 HOMO: -6.87632 LUMO: -0.77825 factor:1 | 1 (-0.45489) | -1 | -1 |
| G: -5684.20830 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.27119 HOMO: -6.45998 LUMO: -0.31565 factor:1 | -1 (0.30281) | -1 | -1 |
| G: -5684.20830 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.23652 HOMO: -7.51306 LUMO: 0.05714 factor:1 | -1 (0.33748) | 1 | 1 |
| G: -5684.20830 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.43051 HOMO: -6.86271 LUMO: -0.00816 factor:1 | -1 (0.14349) | -1 | -1 |
| G: -5684.20830 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.24537 HOMO: -6.43277 LUMO: -1.07485 factor:1 | -1 (0.32863) | -1 | -1 |
| G: -5684.20830 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.78916 HOMO: -6.78108 LUMO: -0.81362 factor:1 | 1 (-0.21516) | -1 | -1 |
| G: -5684.20830 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.43111 HOMO: -6.88448 LUMO: 1.21907 factor:1 | -1 (0.14289) | -1 | -1 |
| G: -5684.20830 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.55547 HOMO: -6.97700 LUMO: 1.44765 factor:1 | -1 (0.01853) | -1 | -1 |
| G: -5684.20830 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.00037 HOMO: -6.89537 LUMO: 2.12249 factor:1 | 1 (-0.42638) | -1 | -1 |
| G: -5684.20830 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.04710 HOMO: -6.28311 LUMO: 1.45037 factor:1 | 1 (-0.47310) | -1 | -1 |
| G: -5684.20830 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.56747 HOMO: -6.55522 LUMO: 1.39867 factor:1 | -1 (0.00653) | -1 | -1 |
| G: -5684.20830 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.08420 HOMO: -6.46815 LUMO: 1.50207 factor:1 | -1 (1.48980) | -1 | -1 |
| G: -5684.20830 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11946.89051 HOMO: -6.43549 LUMO: 2.17419 factor:1 | -1 (1.68349) | -1 | -1 |
| G: -5684.20830 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.09960 HOMO: -6.99333 LUMO: 1.87214 factor:1 | -1 (1.47439) | -1 | -1 |
| G: -5684.20830 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.06526 HOMO: -6.65591 LUMO: 1.37962 factor:1 | -1 (1.50874) | -1 | -1 |
| G: -5684.20830 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11946.98094 HOMO: -6.82734 LUMO: 1.55649 factor:1 | -1 (1.59306) | -1 | -1 |
| G: -5684.20830 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.06746 HOMO: -6.71849 LUMO: 1.36057 factor:1 | -1 (0.50654) | -1 | -1 |
| G: -5684.20830 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.84707 HOMO: -6.79468 LUMO: 1.82044 factor:1 | -1 (0.72692) | -1 | -1 |
| G: -5684.20830 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.48100 HOMO: -6.61237 LUMO: 1.15104 factor:1 | -1 (1.09300) | -1 | -1 |
| G: -5684.20830 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.68413 HOMO: -6.62053 LUMO: 2.33474 factor:1 | -1 (0.88987) | -1 | -1 |
| G: -5684.20830 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.84648 HOMO: -6.55794 LUMO: 1.65717 factor:1 | -1 (0.72752) | -1 | -1 |
| G: -5684.20830 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.08290 HOMO: -6.85999 LUMO: 2.03813 factor:1 | -1 (1.49110) | -1 | -1 |
| G: -5684.20830 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11946.87386 HOMO: -6.45726 LUMO: 1.28438 factor:1 | -1 (1.70014) | -1 | -1 |
| G: -5684.20830 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.16483 HOMO: -6.23685 LUMO: 1.93201 factor:1 | -1 (1.40917) | -1 | -1 |
| G: -5684.20830 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11946.93898 HOMO: -7.06680 LUMO: 1.86942 factor:1 | -1 (1.63502) | 1 | 1 |
| G: -5684.20830 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11946.11855 HOMO: -6.89537 LUMO: 2.17147 factor:1 | -1 (2.45545) | -1 | -1 |
| G: -5684.20830 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.46201 HOMO: -6.80013 LUMO: 1.78779 factor:1 | -1 (1.11199) | -1 | -1 |
| G: -5684.20830 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.59763 HOMO: -6.45726 LUMO: 1.58370 factor:1 | -1 (0.97637) | -1 | -1 |
| G: -5684.20830 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.20551 HOMO: -6.52529 LUMO: 1.71976 factor:1 | -1 (1.36849) | -1 | -1 |
| G: -5684.20830 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.08124 HOMO: -7.22462 LUMO: -1.18642 factor:1 | -1 (1.49276) | 1 | 1 |
| G: -5684.20830 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.10184 HOMO: -7.18381 LUMO: -0.78641 factor:1 | -1 (1.47216) | 1 | 1 |
| G: -5684.20830 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.75839 HOMO: -6.93346 LUMO: 1.65717 factor:1 | -1 (0.81561) | -1 | -1 |
| G: -5684.20830 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11946.88360 HOMO: -6.41644 LUMO: 1.78235 factor:1 | -1 (1.69040) | -1 | -1 |
| G: -5684.20830 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11946.96069 HOMO: -6.59876 LUMO: 1.83677 factor:1 | -1 (1.61331) | -1 | -1 |
| G: -5684.20830 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11946.75650 HOMO: -6.35658 LUMO: 1.59731 factor:1 | -1 (1.81750) | -1 | -1 |
| G: -5684.20830 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.20423 HOMO: -6.60692 LUMO: 1.66534 factor:1 | -1 (1.36977) | -1 | -1 |
| G: -5684.20830 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.07256 HOMO: -6.83006 LUMO: 2.11705 factor:1 | -1 (1.50144) | -1 | -1 |
| G: -5684.20830 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11946.84678 HOMO: -6.89264 LUMO: 1.30070 factor:1 | -1 (1.72722) | -1 | -1 |
| G: -5684.20830 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11946.66912 HOMO: -6.90081 LUMO: 2.05174 factor:1 | -1 (1.90488) | -1 | -1 |
| G: -5684.20830 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11946.67421 HOMO: -6.74842 LUMO: 1.96194 factor:1 | -1 (1.89979) | -1 | -1 |
| G: -5684.20830 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11946.86069 HOMO: -6.58516 LUMO: 1.30887 factor:1 | -1 (1.71331) | -1 | -1 |
| G: -5684.20830 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.99535 HOMO: -7.00965 LUMO: 2.08167 factor:1 | -1 (0.57865) | -1 | -1 |
| G: -5684.20830 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11946.94091 HOMO: -6.86815 LUMO: 2.29664 factor:1 | -1 (1.63309) | -1 | -1 |
| G: -5684.20830 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.04898 HOMO: -6.39740 LUMO: 2.02725 factor:1 | -1 (0.52502) | -1 | -1 |
| G: -5684.20830 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.99790 HOMO: -5.95929 LUMO: 1.62724 factor:1 | 1 (-0.42390) | -1 | -1 |
| G: -5684.20830 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.20504 HOMO: -6.71849 LUMO: 1.34696 factor:1 | -1 (0.36896) | -1 | -1 |
| G: -5684.20830 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.35895 HOMO: -7.26816 LUMO: 1.74153 factor:1 | -1 (0.21505) | 1 | 1 |
| G: -5684.20830 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11946.29826 HOMO: -6.90897 LUMO: 1.71432 factor:1 | -1 (2.27574) | -1 | -1 |
| G: -5684.20830 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11946.25605 HOMO: -6.70489 LUMO: 1.91568 factor:1 | -1 (2.31795) | -1 | -1 |
| G: -5684.20830 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11945.90015 HOMO: -6.83278 LUMO: 1.61908 factor:1 | -1 (2.67385) | -1 | -1 |
| G: -5684.20830 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.09433 HOMO: -7.17292 LUMO: 1.95378 factor:1 | -1 (1.47967) | 1 | -1 |
| G: -5684.20830 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11946.97786 HOMO: -6.53345 LUMO: 1.74153 factor:1 | -1 (1.59614) | -1 | -1 |
| G: -5684.20830 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11946.99103 HOMO: -6.53073 LUMO: 1.51023 factor:1 | -1 (1.58297) | -1 | -1 |
| G: -5684.20830 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.09601 HOMO: -6.93346 LUMO: 2.22861 factor:1 | -1 (1.47799) | -1 | -1 |
| G: -5684.20830 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.00319 HOMO: -6.47903 LUMO: 2.05446 factor:1 | -1 (1.57080) | -1 | -1 |
| G: -5684.20830 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.00812 HOMO: -6.88992 LUMO: 1.57010 factor:1 | -1 (1.56588) | -1 | -1 |
| G: -5684.20830 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.14946 HOMO: -6.07358 LUMO: 1.95922 factor:1 | -1 (1.42454) | -1 | -1 |
| G: -5684.20830 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.03051 HOMO: -6.75114 LUMO: 2.18780 factor:1 | -1 (1.54348) | -1 | -1 |
| G: -5684.20830 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.25732 HOMO: -6.96339 LUMO: 1.70071 factor:1 | -1 (1.31668) | -1 | -1 |
| G: -5684.20830 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.41517 HOMO: -7.14843 LUMO: 1.82588 factor:1 | -1 (1.15882) | 1 | -1 |
| G: -5684.20830 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.71752 HOMO: -6.96339 LUMO: 2.29392 factor:1 | -1 (0.85648) | -1 | -1 |
| G: -5684.20830 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.04049 HOMO: -6.81645 LUMO: 2.39732 factor:1 | -1 (0.53351) | -1 | -1 |
| G: -5684.20830 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.87967 HOMO: -6.48447 LUMO: 1.24084 factor:1 | -1 (0.69433) | -1 | -1 |
| G: -5684.20830 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.68657 HOMO: -7.14843 LUMO: 2.01092 factor:1 | 1 (-0.11257) | 1 | -1 |
| G: -5684.20830 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.35742 HOMO: -7.20013 LUMO: -0.34286 factor:1 | -1 (0.21658) | 1 | -1 |
| G: -5684.20830 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.18918 HOMO: -6.97700 LUMO: -0.15238 factor:1 | -1 (0.38482) | -1 | -1 |
| G: -5684.20830 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.99187 HOMO: -7.07768 LUMO: -0.26123 factor:1 | -1 (0.58213) | 1 | -1 |
| G: -5684.20830 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.21582 HOMO: -6.99333 LUMO: -0.41361 factor:1 | -1 (0.35818) | -1 | -1 |
| G: -5684.20830 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11945.81531 HOMO: -6.84638 LUMO: -0.40273 factor:1 | -1 (2.75869) | -1 | -1 |
| G: -5684.20830 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11945.98152 HOMO: -6.83822 LUMO: -0.26939 factor:1 | -1 (2.59248) | -1 | -1 |
| G: -5684.20830 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11946.12625 HOMO: -6.75931 LUMO: -0.93879 factor:1 | -1 (2.44775) | -1 | -1 |
| G: -5684.20830 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11946.90044 HOMO: -6.79468 LUMO: -0.39729 factor:1 | -1 (1.67355) | -1 | -1 |
| G: -5684.20830 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11946.64928 HOMO: -6.93890 LUMO: 0.43266 factor:1 | -1 (1.92472) | -1 | -1 |
| G: -5684.20830 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11946.89402 HOMO: -7.08040 LUMO: -0.85716 factor:1 | -1 (1.67998) | 1 | 1 |
| G: -5684.20830 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.01955 HOMO: -6.70216 LUMO: -1.41499 factor:1 | -1 (1.55445) | -1 | -1 |
| G: -5684.20830 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11946.98722 HOMO: -6.63686 LUMO: -0.52790 factor:1 | -1 (1.58678) | -1 | -1 |
| G: -5684.20830 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11946.98521 HOMO: -6.75114 LUMO: -0.13334 factor:1 | -1 (1.58879) | -1 | -1 |
| G: -5684.20830 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11946.98189 HOMO: -6.94435 LUMO: -0.24490 factor:1 | -1 (1.59211) | -1 | -1 |
| G: -5684.20830 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.04398 HOMO: -6.74298 LUMO: -0.84627 factor:1 | -1 (1.53001) | -1 | -1 |
| G: -5684.20830 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.78854 HOMO: -7.15932 LUMO: 0.22041 factor:1 | -1 (0.78546) | 1 | 1 |
| G: -5684.20830 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.58084 HOMO: -6.90081 LUMO: -1.16737 factor:1 | -1 (0.99316) | -1 | -1 |
| G: -5684.20830 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11946.74575 HOMO: -7.04775 LUMO: -0.84355 factor:1 | -1 (1.82825) | -1 | -1 |
| G: -5684.20830 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.00796 HOMO: -7.17020 LUMO: -1.31159 factor:1 | -1 (1.56604) | 1 | 1 |
| G: -5684.20830 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.97391 HOMO: -7.14571 LUMO: -0.46259 factor:1 | -1 (0.60009) | 1 | 1 |
| G: -5684.20830 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.99391 HOMO: -7.45048 LUMO: -0.91158 factor:1 | -1 (0.58009) | 1 | 1 |
| G: -5684.20830 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.75863 HOMO: -6.87360 LUMO: -0.82995 factor:1 | 1 (-0.18463) | -1 | -1 |
| G: -5684.20830 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.24618 HOMO: -7.43415 LUMO: -0.65307 factor:1 | -1 (0.32782) | 1 | 1 |
| G: -5684.20830 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.16313 HOMO: -7.47225 LUMO: -0.77280 factor:1 | -1 (0.41086) | 1 | 1 |
| G: -5684.20830 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.24967 HOMO: -6.86271 LUMO: -0.83811 factor:1 | -1 (0.32433) | -1 | -1 |
| G: -5684.20830 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.15021 HOMO: -7.53483 LUMO: -0.66124 factor:1 | -1 (0.42379) | 1 | 1 |
| G: -5684.20830 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.48007 HOMO: -7.45864 LUMO: -1.08301 factor:1 | -1 (0.09393) | 1 | 1 |
| G: -5684.20830 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.65951 HOMO: -7.24639 LUMO: -1.19186 factor:1 | -1 (0.91449) | 1 | 1 |
| G: -5684.20830 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.93695 HOMO: -7.54844 LUMO: -0.96873 factor:1 | -1 (0.63705) | 1 | 1 |
| G: -5684.20830 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.91287 HOMO: -7.12666 LUMO: -0.01633 factor:1 | -1 (0.66113) | 1 | 1 |
| G: -5684.20830 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.35925 HOMO: -6.77291 LUMO: -0.70477 factor:1 | -1 (0.21475) | -1 | -1 |
| G: -5684.20830 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.04704 HOMO: -6.76475 LUMO: -1.15921 factor:1 | 1 (-0.47304) | -1 | -1 |
| G: -5684.20830 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.29340 HOMO: -5.37697 LUMO: -0.56600 factor:1 | -1 (0.28060) | -1 | -1 |
| G: -5684.20830 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.30382 HOMO: -6.62053 LUMO: -1.75513 factor:1 | -1 (0.27018) | -1 | -1 |
| G: -5684.20830 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.05728 HOMO: -6.60420 LUMO: -1.74697 factor:1 | -1 (0.51672) | -1 | -1 |
| G: -5684.20830 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.44817 HOMO: -6.84366 LUMO: -0.94968 factor:1 | -1 (0.12583) | -1 | -1 |
| G: -5684.20830 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.79076 HOMO: -6.96884 LUMO: -2.11977 factor:1 | 1 (-0.21677) | -1 | -1 |
| G: -5684.20830 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.80668 HOMO: -6.80829 LUMO: 0.56055 factor:1 | 1 (-0.23268) | -1 | -1 |
| G: -5684.20830 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11946.98145 HOMO: -7.02326 LUMO: 0.11429 factor:1 | -1 (1.59255) | -1 | -1 |
| G: -5684.20830 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.01604 HOMO: -7.40966 LUMO: 0.18232 factor:1 | -1 (1.55796) | 1 | 1 |
| G: -5684.20830 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.13084 HOMO: -6.34570 LUMO: 0.41089 factor:1 | -1 (1.44316) | -1 | -1 |
| G: -5684.20830 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.05887 HOMO: -6.78924 LUMO: 0.49525 factor:1 | -1 (1.51513) | -1 | -1 |
| G: -5684.20830 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11946.94251 HOMO: -6.87632 LUMO: 0.44082 factor:1 | -1 (1.63149) | -1 | -1 |
| G: -5684.20830 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.61999 HOMO: -6.69944 LUMO: 1.20546 factor:1 | -1 (0.95400) | -1 | -1 |
| G: -5684.20830 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.05396 HOMO: -6.83006 LUMO: 1.28982 factor:1 | -1 (0.52004) | -1 | -1 |
| G: -5684.20830 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.90585 HOMO: -7.78246 LUMO: 0.20681 factor:1 | -1 (0.66815) | 1 | 1 |
| G: -5684.20830 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.86438 HOMO: -6.55794 LUMO: -1.65173 factor:1 | -1 (0.70962) | -1 | -1 |
| G: -5684.20830 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.26812 HOMO: -6.77564 LUMO: -1.14560 factor:1 | -1 (0.30588) | -1 | -1 |
| G: -5684.20830 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.34447 HOMO: -7.46680 LUMO: -1.18097 factor:1 | -1 (0.22953) | 1 | 1 |
| G: -5684.20830 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.97848 HOMO: -6.88176 LUMO: -1.24900 factor:1 | -1 (0.59552) | -1 | -1 |
| G: -5684.20830 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.23032 HOMO: -7.28177 LUMO: -0.42178 factor:1 | -1 (0.34368) | 1 | 1 |
| G: -5684.20830 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.01998 HOMO: -7.71715 LUMO: 0.19592 factor:1 | -1 (0.55402) | 1 | 1 |
| G: -5684.20830 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.03481 HOMO: -7.02326 LUMO: -1.40683 factor:1 | -1 (1.53918) | -1 | -1 |
| G: -5684.20830 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11946.88820 HOMO: -7.27088 LUMO: -1.07485 factor:1 | -1 (1.68580) | 1 | 1 |
| G: -5684.20830 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.01136 HOMO: -7.17020 LUMO: -0.49525 factor:1 | -1 (1.56264) | 1 | 1 |
| G: -5684.20830 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11946.86787 HOMO: -7.15932 LUMO: 0.02721 factor:1 | -1 (1.70613) | 1 | 1 |
| G: -5684.20830 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.15797 HOMO: -7.00693 LUMO: -0.83267 factor:1 | -1 (1.41603) | -1 | -1 |
| G: -5684.20830 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.07990 HOMO: -6.86543 LUMO: -0.10340 factor:1 | -1 (1.49410) | -1 | -1 |
| G: -5684.20830 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11946.79816 HOMO: -7.11850 LUMO: -0.08980 factor:1 | -1 (1.77584) | 1 | 1 |
| G: -5684.20830 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11946.69633 HOMO: -6.87087 LUMO: -0.88981 factor:1 | -1 (1.87767) | -1 | -1 |
| G: -5684.20830 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.07343 HOMO: -7.08857 LUMO: -1.27077 factor:1 | -1 (1.50057) | 1 | 1 |
| G: -5684.20830 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11946.90896 HOMO: -6.79468 LUMO: -0.81906 factor:1 | -1 (1.66504) | -1 | -1 |
| G: -5684.20830 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11946.99190 HOMO: -6.86815 LUMO: -0.89798 factor:1 | -1 (1.58210) | -1 | -1 |
| G: -5684.20830 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.70547 HOMO: -6.78652 LUMO: -2.00548 factor:1 | -1 (0.86853) | -1 | -1 |
| G: -5684.20830 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.77573 HOMO: -6.75114 LUMO: -0.08436 factor:1 | -1 (0.79827) | -1 | -1 |
| G: -5684.20830 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.69267 HOMO: -6.55794 LUMO: 0.52790 factor:1 | 1 (-0.11867) | -1 | -1 |
| G: -5684.20830 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.28885 HOMO: -7.17836 LUMO: 0.28300 factor:1 | -1 (0.28515) | 1 | -1 |
| G: -5684.20830 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.76669 HOMO: -7.35796 LUMO: -0.77552 factor:1 | -1 (0.80731) | 1 | 1 |
| G: -5684.20830 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.08234 HOMO: -7.23551 LUMO: -1.17553 factor:1 | -1 (0.49166) | 1 | 1 |
| G: -5684.20830 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.98338 HOMO: -7.07496 LUMO: -1.14288 factor:1 | -1 (0.59062) | 1 | 1 |
| G: -5684.20830 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.34431 HOMO: -6.70489 LUMO: -0.83539 factor:1 | -1 (0.22969) | -1 | -1 |
| G: -5684.20830 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.79442 HOMO: -6.59604 LUMO: -0.89798 factor:1 | -1 (0.77958) | -1 | -1 |
| G: -5684.20830 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.88408 HOMO: -6.94162 LUMO: -1.22451 factor:1 | -1 (0.68992) | -1 | -1 |
| G: -5684.20830 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.73864 HOMO: -6.68040 LUMO: 0.22041 factor:1 | -1 (0.83536) | -1 | -1 |
| G: -5684.20830 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.66272 HOMO: -6.88176 LUMO: 0.11157 factor:1 | -1 (0.91128) | -1 | -1 |
| G: -5684.20830 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.56742 HOMO: -6.91713 LUMO: 1.27621 factor:1 | -1 (1.00658) | -1 | -1 |
| G: -5684.20830 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11946.92020 HOMO: -6.77836 LUMO: 1.01226 factor:1 | -1 (1.65380) | -1 | -1 |
| G: -5684.20830 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11946.62907 HOMO: -7.14571 LUMO: 1.48574 factor:1 | -1 (1.94493) | 1 | 1 |
| G: -5684.20830 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11946.93503 HOMO: -6.96884 LUMO: 1.48574 factor:1 | -1 (1.63897) | -1 | -1 |
| G: -5684.20830 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11946.99979 HOMO: -7.24367 LUMO: 1.28438 factor:1 | -1 (1.57421) | 1 | 1 |
| G: -5684.20830 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.11090 HOMO: -7.10489 LUMO: 1.29526 factor:1 | -1 (1.46310) | 1 | 1 |
| G: -5684.20830 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.19308 HOMO: -7.07224 LUMO: 1.29254 factor:1 | -1 (1.38092) | 1 | 1 |
| G: -5684.20830 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.45773 HOMO: -7.12938 LUMO: 0.49253 factor:1 | -1 (1.11627) | 1 | 1 |
| G: -5684.20830 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.67972 HOMO: -7.33619 LUMO: 1.45581 factor:1 | -1 (0.89427) | 1 | 1 |
| G: -5684.20830 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.46184 HOMO: -6.87904 LUMO: -0.14422 factor:1 | -1 (1.11216) | -1 | -1 |
| G: -5684.20830 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11946.71982 HOMO: -6.81917 LUMO: 0.50341 factor:1 | -1 (1.85418) | -1 | -1 |
| G: -5684.20830 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11946.88785 HOMO: -7.27905 LUMO: 0.13606 factor:1 | -1 (1.68615) | 1 | -1 |
| G: -5684.20830 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11946.97253 HOMO: -6.87904 LUMO: -0.09796 factor:1 | -1 (1.60147) | -1 | -1 |
| G: -5684.20830 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11946.91813 HOMO: -7.33891 LUMO: 0.03810 factor:1 | -1 (1.65587) | 1 | 1 |
| G: -5684.20830 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11946.87965 HOMO: -6.98516 LUMO: 0.98233 factor:1 | -1 (1.69434) | -1 | -1 |
| G: -5684.20830 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.88278 HOMO: -6.94162 LUMO: 0.86804 factor:1 | -1 (0.69122) | -1 | -1 |
| G: -5684.20830 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.81502 HOMO: -7.37701 LUMO: 0.05442 factor:1 | -1 (0.75898) | 1 | 1 |
| G: -5684.20830 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.81224 HOMO: -7.04775 LUMO: 0.43266 factor:1 | -1 (0.76176) | -1 | -1 |
| G: -5684.20830 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.60010 HOMO: -7.47497 LUMO: 0.31837 factor:1 | -1 (0.97390) | 1 | 1 |
| G: -5684.20830 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.82261 HOMO: -6.62053 LUMO: 0.13061 factor:1 | -1 (0.75139) | -1 | -1 |
| G: -5684.20830 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.25855 HOMO: -6.44366 LUMO: -0.04354 factor:1 | -1 (1.31545) | -1 | -1 |
| G: -5684.20830 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.41705 HOMO: -6.40284 LUMO: 0.68301 factor:1 | -1 (1.15695) | -1 | -1 |
| G: -5684.20830 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.01217 HOMO: -6.73754 LUMO: 0.36735 factor:1 | -1 (1.56182) | -1 | -1 |
| G: -5684.20830 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.03245 HOMO: -6.85455 LUMO: 0.23946 factor:1 | -1 (1.54155) | -1 | -1 |
| G: -5684.20830 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.30154 HOMO: -6.93346 LUMO: 0.24762 factor:1 | -1 (1.27246) | -1 | -1 |
| G: -5684.20830 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.84920 HOMO: -6.85455 LUMO: 0.17687 factor:1 | -1 (0.72480) | -1 | -1 |
| G: -5684.20830 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.81997 HOMO: -6.62325 LUMO: 0.69933 factor:1 | -1 (0.75403) | -1 | -1 |
| G: -5684.20830 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.89540 HOMO: -6.43005 LUMO: 0.50069 factor:1 | -1 (0.67860) | -1 | -1 |
| G: -5684.20830 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.41297 HOMO: -6.56883 LUMO: 0.22858 factor:1 | -1 (1.16103) | -1 | -1 |
| G: -5684.20830 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.18558 HOMO: -6.78380 LUMO: 0.54967 factor:1 | -1 (0.38842) | -1 | -1 |
| G: -5684.20830 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.28550 HOMO: -7.35524 LUMO: 0.00272 factor:1 | -1 (0.28850) | 1 | 1 |
| G: -5684.20830 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.13410 HOMO: -7.27360 LUMO: 0.08436 factor:1 | -1 (0.43990) | 1 | 1 |
| G: -5684.20830 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11945.53982 HOMO: -7.44504 LUMO: -0.96056 factor:1 | -1 (3.03418) | 1 | 1 |
| G: -5684.20830 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11945.82105 HOMO: -7.27360 LUMO: 0.29933 factor:1 | -1 (2.75295) | 1 | 1 |
| G: -5684.20830 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11945.83128 HOMO: -7.09129 LUMO: 0.41089 factor:1 | -1 (2.74272) | 1 | 1 |
| G: -5684.20830 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11946.88066 HOMO: -6.93618 LUMO: 0.36463 factor:1 | -1 (1.69334) | -1 | -1 |
| G: -5684.20830 HOMO: -7.26000 LUMO: -3.02863 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11946.78221 HOMO: -7.65728 LUMO: 0.20136 factor:1 | -1 (1.79179) | 1 | 1 |
| G: -5684.20830 HOMO: -7.26000 LUMO: -3.02863 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11946.64754 HOMO: -6.90353 LUMO: -0.92791 factor:1 | -1 (1.92646) | -1 | -1 |
| G: -5684.20830 HOMO: -7.26000 LUMO: -3.02863 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11945.91202 HOMO: -6.82462 LUMO: -1.18370 factor:1 | -1 (2.66198) | -1 | -1 |
| G: -5684.20830 HOMO: -7.26000 LUMO: -3.02863 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11946.59402 HOMO: -7.09129 LUMO: -0.13334 factor:1 | -1 (1.97998) | 1 | 1 |
| G: -5684.20830 HOMO: -7.26000 LUMO: -3.02863 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.32056 HOMO: -7.40966 LUMO: -1.06941 factor:1 | -1 (1.25344) | 1 | 1 |
| G: -5684.20830 HOMO: -7.26000 LUMO: -3.02863 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.22336 HOMO: -7.24367 LUMO: -1.00954 factor:1 | -1 (1.35064) | 1 | 1 |
| G: -5684.20830 HOMO: -7.26000 LUMO: -3.02863 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.39692 HOMO: -7.51851 LUMO: 0.09796 factor:1 | -1 (1.17708) | 1 | 1 |
| G: -5684.20830 HOMO: -7.26000 LUMO: -3.02863 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.88375 HOMO: -7.48857 LUMO: -0.07619 factor:1 | -1 (0.69024) | 1 | 1 |
| G: -5684.20830 HOMO: -7.26000 LUMO: -3.02863 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.68775 HOMO: -6.53345 LUMO: 1.09390 factor:1 | -1 (0.88625) | -1 | -1 |
| G: -5684.20830 HOMO: -7.26000 LUMO: -3.02863 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.78637 HOMO: -7.21918 LUMO: 0.08436 factor:1 | -1 (0.78763) | 1 | 1 |
| G: -5684.20830 HOMO: -7.26000 LUMO: -3.02863 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.64974 HOMO: -7.38789 LUMO: 1.02587 factor:1 | -1 (0.92426) | 1 | -1 |
| G: -5684.20830 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11946.63736 HOMO: -6.83550 LUMO: -0.67484 factor:1 | -1 (1.93663) | -1 | -1 |
| G: -5684.20830 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11946.78243 HOMO: -7.04231 LUMO: 0.54151 factor:1 | -1 (1.79157) | -1 | -1 |
| G: -5684.20830 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.64544 HOMO: -6.79740 LUMO: 1.91296 factor:1 | -1 (0.92856) | 1 | 1 |
| G: -5684.20830 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.65923 HOMO: -7.35796 LUMO: -1.04220 factor:1 | -1 (0.91477) | -1 | -1 |
| G: -5684.20830 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.72065 HOMO: -6.62597 LUMO: -0.44082 factor:1 | -1 (0.85335) | -1 | -1 |
| G: -5684.20830 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.53178 HOMO: -6.45182 LUMO: -0.20409 factor:1 | -1 (1.04222) | -1 | -1 |
| G: -5684.20830 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.81706 HOMO: -6.51168 LUMO: -0.23130 factor:1 | -1 (0.75694) | -1 | -1 |
| G: -5684.20830 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.88536 HOMO: -7.14027 LUMO: 0.49797 factor:1 | -1 (0.68864) | -1 | -1 |
| G: -5684.20830 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.59665 HOMO: -7.55660 LUMO: 0.24762 factor:1 | -1 (0.97735) | -1 | -1 |
| G: -5684.20830 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.49194 HOMO: -6.88992 LUMO: -0.64763 factor:1 | -1 (1.08206) | -1 | -1 |
| G: -5684.20830 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.02575 HOMO: -6.72665 LUMO: -0.45987 factor:1 | -1 (1.54825) | -1 | -1 |
| G: -5684.20830 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11946.93742 HOMO: -6.72121 LUMO: -0.58232 factor:1 | -1 (1.63657) | -1 | -1 |
| G: -5684.20830 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11945.96075 HOMO: -7.26816 LUMO: 0.32926 factor:1 | -1 (2.61325) | -1 | -1 |
| G: -5684.20830 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11946.91380 HOMO: -6.57155 LUMO: -0.53606 factor:1 | -1 (1.66019) | -1 | -1 |
| G: -5684.20830 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.24600 HOMO: -6.50896 LUMO: -0.43810 factor:1 | -1 (1.32800) | -1 | -1 |
| G: -5684.20830 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11946.66104 HOMO: -6.73210 LUMO: -0.51430 factor:1 | -1 (1.91296) | -1 | -1 |
| G: -5684.20830 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11946.61785 HOMO: -6.77019 LUMO: -0.62858 factor:1 | -1 (1.95614) | -1 | -1 |
| G: -5684.20830 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11946.87914 HOMO: -6.82462 LUMO: -0.67484 factor:1 | -1 (1.69486) | -1 | -1 |
| G: -5684.20830 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11946.86648 HOMO: -6.79740 LUMO: -0.55511 factor:1 | -1 (1.70751) | -1 | -1 |
| G: -5684.20830 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11946.76335 HOMO: -6.79740 LUMO: -0.67756 factor:1 | -1 (1.81065) | -1 | -1 |
| G: -5684.20830 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.00627 HOMO: -6.75114 LUMO: -0.55239 factor:1 | 1 (-1.43227) | -1 | -1 |
| G: -5684.20830 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.01060 HOMO: -6.49536 LUMO: -0.25307 factor:1 | 1 (-1.43660) | -1 | -1 |
| G: -5684.20830 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.03384 HOMO: -6.48992 LUMO: -0.25034 factor:1 | 1 (-1.45984) | -1 | -1 |
| G: -5684.20830 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.23008 HOMO: -6.52801 LUMO: -0.28028 factor:1 | 1 (-1.65608) | -1 | -1 |
| G: -5684.20830 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.79247 HOMO: -7.22462 LUMO: 0.52518 factor:1 | 1 (-1.21847) | -1 | -1 |
| G: -5684.20830 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.11740 HOMO: -6.59332 LUMO: -0.27211 factor:1 | 1 (-1.54340) | -1 | -1 |
| G: -5684.20830 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.66477 HOMO: -6.57427 LUMO: -0.16871 factor:1 | 1 (-1.09077) | -1 | -1 |
| G: -5684.20830 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.88406 HOMO: -6.71033 LUMO: 1.59187 factor:1 | 1 (-1.31006) | 1 | 1 |
| G: -5684.20830 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.27012 HOMO: -6.72121 LUMO: 2.00004 factor:1 | 1 (-0.69612) | 1 | 1 |
| G: -5684.20830 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.27408 HOMO: -6.61509 LUMO: 1.55921 factor:1 | 1 (-1.70009) | -1 | -1 |
| G: -5684.20830 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.21520 HOMO: -6.55250 LUMO: 1.73064 factor:1 | 1 (-1.64120) | -1 | -1 |
| G: -5684.20830 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.77484 HOMO: -6.66135 LUMO: 2.02181 factor:1 | 1 (-1.20084) | 1 | 1 |
| G: -5684.20830 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.05933 HOMO: -6.84911 LUMO: 1.98099 factor:1 | 1 (-1.48533) | 1 | 1 |
| G: -5684.20830 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.21360 HOMO: -6.66679 LUMO: 1.98371 factor:1 | 1 (-0.63960) | 1 | 1 |
| G: -5684.20830 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.30777 HOMO: -6.67495 LUMO: 2.04085 factor:1 | 1 (-1.73377) | 1 | 1 |
| G: -5684.20830 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.48956 HOMO: -6.89809 LUMO: 1.95106 factor:1 | -1 (0.08444) | 1 | 1 |
| G: -5684.20830 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.63824 HOMO: -6.50352 LUMO: 1.88847 factor:1 | 1 (-1.06424) | -1 | -1 |
| G: -5684.20830 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.88899 HOMO: -6.93618 LUMO: 2.00004 factor:1 | 1 (-1.31499) | 1 | 1 |
| G: -5684.20830 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.20026 HOMO: -6.50896 LUMO: 1.73609 factor:1 | 1 (-1.62626) | -1 | -1 |
| G: -5684.20830 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.29162 HOMO: -6.69672 LUMO: 2.37283 factor:1 | 1 (-0.71762) | 1 | 1 |
| G: -5684.20830 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.38976 HOMO: -6.65591 LUMO: 2.20684 factor:1 | 1 (-1.81576) | 1 | 1 |
| G: -5684.20830 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.48454 HOMO: -6.23957 LUMO: 1.78507 factor:1 | 1 (-1.91054) | -1 | -1 |
| G: -5684.20830 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.81405 HOMO: -6.35114 LUMO: 1.92112 factor:1 | 1 (-1.24005) | -1 | -1 |
| G: -5684.20830 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.99680 HOMO: -6.53617 LUMO: 1.75241 factor:1 | 1 (-1.42280) | -1 | -1 |
| G: -5684.20830 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.26339 HOMO: -6.60420 LUMO: 1.78779 factor:1 | 1 (-1.68939) | 1 | 1 |
| G: -5684.20830 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.31738 HOMO: -7.40422 LUMO: -0.97145 factor:1 | 1 (-1.74338) | -1 | -1 |
| G: -5684.20830 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.91850 HOMO: -6.80013 LUMO: -0.69117 factor:1 | 1 (-2.34451) | -1 | -1 |
| G: -5684.20830 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.86736 HOMO: -6.68040 LUMO: -0.47076 factor:1 | 1 (-1.29336) | -1 | -1 |
| G: -5684.20830 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.84419 HOMO: -7.20285 LUMO: -0.66124 factor:1 | 1 (-2.27019) | -1 | -1 |
| G: -5684.20830 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.27400 HOMO: -6.82734 LUMO: -0.60137 factor:1 | 1 (-1.70000) | -1 | -1 |
| G: -5684.20830 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.15786 HOMO: -7.18653 LUMO: 0.59321 factor:1 | 1 (-1.58387) | -1 | -1 |
| G: -5684.20830 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.90006 HOMO: -7.29265 LUMO: 0.48164 factor:1 | 1 (-1.32607) | -1 | -1 |
| G: -5684.20830 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.28821 HOMO: -6.63414 LUMO: -0.25034 factor:1 | 1 (-1.71421) | -1 | -1 |
| G: -5684.20830 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.72082 HOMO: -7.20285 LUMO: 0.53879 factor:1 | 1 (-1.14682) | -1 | -1 |
| G: -5684.20830 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.63127 HOMO: -6.46815 LUMO: -0.21769 factor:1 | 1 (-1.05727) | -1 | -1 |
| G: -5684.20830 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.72493 HOMO: -6.57971 LUMO: -0.18776 factor:1 | 1 (-1.15093) | -1 | -1 |
| G: -5684.20830 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.49557 HOMO: -6.90897 LUMO: 1.91296 factor:1 | 1 (-0.92157) | 1 | 1 |
| G: -5684.20830 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.67877 HOMO: -6.67495 LUMO: 2.04358 factor:1 | 1 (-2.10477) | 1 | 1 |
| G: -5684.20830 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.53195 HOMO: -6.94162 LUMO: 1.73881 factor:1 | 1 (-0.95795) | 1 | 1 |
| G: -5684.20830 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.88975 HOMO: -6.73482 LUMO: 1.95922 factor:1 | 1 (-1.31575) | 1 | 1 |
| G: -5684.20830 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.12010 HOMO: -6.70489 LUMO: 2.04358 factor:1 | 1 (-1.54610) | 1 | 1 |
| G: -5684.20830 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.97212 HOMO: -7.04231 LUMO: 1.79323 factor:1 | 1 (-1.39812) | 1 | 1 |
| G: -5684.20830 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.05525 HOMO: -6.68584 LUMO: 1.60275 factor:1 | 1 (-1.48125) | 1 | 1 |
| G: -5684.20830 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.90627 HOMO: -6.40556 LUMO: 1.45581 factor:1 | 1 (-1.33227) | -1 | -1 |
| G: -5684.20830 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.96537 HOMO: -6.94979 LUMO: 2.16603 factor:1 | 1 (-1.39137) | 1 | 1 |
| G: -5684.20830 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.98262 HOMO: -6.84911 LUMO: 1.89935 factor:1 | 1 (-1.40862) | 1 | 1 |
| G: -5684.20830 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.96230 HOMO: -6.22052 LUMO: 1.57282 factor:1 | 1 (-1.38830) | -1 | -1 |
| G: -5684.20830 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.07043 HOMO: -6.51168 LUMO: 2.10072 factor:1 | 1 (-1.49644) | -1 | -1 |
| G: -5684.20830 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.10001 HOMO: -7.03686 LUMO: 2.12249 factor:1 | 1 (-1.52601) | 1 | 1 |
| G: -5684.20830 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.06826 HOMO: -6.84094 LUMO: 1.63268 factor:1 | 1 (-1.49426) | 1 | 1 |
| G: -5684.20830 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.13201 HOMO: -6.75387 LUMO: 1.72248 factor:1 | 1 (-1.55802) | 1 | 1 |
| G: -5684.20830 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.08301 HOMO: -6.86271 LUMO: 1.68711 factor:1 | 1 (-1.50901) | 1 | 1 |
| G: -5684.20830 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.11003 HOMO: -6.84094 LUMO: 2.02997 factor:1 | 1 (-1.53603) | 1 | 1 |
| G: -5684.20830 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11951.09900 HOMO: -6.80557 LUMO: 2.02725 factor:1 | 1 (-2.52500) | 1 | 1 |
| G: -5684.20830 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.84012 HOMO: -6.38651 LUMO: 1.53472 factor:1 | 1 (-1.26612) | -1 | -1 |
| G: -5684.20830 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.91258 HOMO: -7.51306 LUMO: 0.28572 factor:1 | 1 (-1.33858) | -1 | -1 |
| G: -5684.20830 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.95367 HOMO: -6.97972 LUMO: -0.74287 factor:1 | 1 (-1.37967) | -1 | -1 |
| G: -5684.20830 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.82926 HOMO: -6.83822 LUMO: -0.65852 factor:1 | 1 (-1.25526) | -1 | -1 |
| G: -5684.20830 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.86270 HOMO: -6.71305 LUMO: -0.49525 factor:1 | 1 (-1.28870) | -1 | -1 |
| G: -5684.20830 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.76613 HOMO: -6.60692 LUMO: -0.22313 factor:1 | 1 (-1.19213) | -1 | -1 |
| G: -5684.20830 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.01852 HOMO: -7.20013 LUMO: 0.55239 factor:1 | 1 (-1.44452) | -1 | -1 |
| G: -5684.20830 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.85802 HOMO: -6.60420 LUMO: -0.28028 factor:1 | 1 (-1.28402) | -1 | -1 |
| G: -5684.20830 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.91726 HOMO: -6.69128 LUMO: -0.30477 factor:1 | 1 (-1.34326) | -1 | -1 |
| G: -5684.20830 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.92292 HOMO: -6.65591 LUMO: -0.25579 factor:1 | 1 (-1.34892) | -1 | -1 |
| G: -5684.20830 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.03220 HOMO: -6.69128 LUMO: 1.70888 factor:1 | 1 (-1.45820) | 1 | 1 |
| G: -5684.20830 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.64610 HOMO: -6.50080 LUMO: 1.87759 factor:1 | 1 (-1.07210) | -1 | -1 |
| G: -5684.20830 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.67786 HOMO: -6.85727 LUMO: 1.99187 factor:1 | 1 (-1.10386) | 1 | 1 |
| G: -5684.20830 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.79691 HOMO: -6.58788 LUMO: 1.79051 factor:1 | 1 (-1.22291) | 1 | 1 |
| G: -5684.20830 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.82907 HOMO: -6.64230 LUMO: 2.16058 factor:1 | 1 (-1.25507) | 1 | 1 |
| G: -5684.20830 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.94692 HOMO: -6.58788 LUMO: 2.10616 factor:1 | 1 (-1.37292) | 1 | 1 |
| G: -5684.20830 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.63663 HOMO: -7.01782 LUMO: 2.13609 factor:1 | 1 (-1.06263) | 1 | 1 |
| G: -5684.20830 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.76831 HOMO: -6.31304 LUMO: 2.31841 factor:1 | 1 (-1.19431) | -1 | -1 |
| G: -5684.20830 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.59552 HOMO: -6.94979 LUMO: 2.07895 factor:1 | 1 (-0.02152) | 1 | 1 |
| G: -5684.20830 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.82904 HOMO: -6.88992 LUMO: 2.28031 factor:1 | 1 (-1.25504) | 1 | 1 |
| G: -5684.20830 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.63786 HOMO: -6.66407 LUMO: 2.07623 factor:1 | 1 (-1.06386) | 1 | 1 |
| G: -5684.20830 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.92763 HOMO: -6.52529 LUMO: 1.70071 factor:1 | 1 (-1.35363) | -1 | -1 |
| G: -5684.20830 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.88877 HOMO: -6.58788 LUMO: 1.57282 factor:1 | 1 (-1.31477) | -1 | -1 |
| G: -5684.20830 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.69892 HOMO: -6.55250 LUMO: 1.95378 factor:1 | 1 (-1.12492) | -1 | -1 |
| G: -5684.20830 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.85663 HOMO: -6.24773 LUMO: 1.77962 factor:1 | 1 (-1.28264) | -1 | -1 |
| G: -5684.20830 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.55282 HOMO: -6.31304 LUMO: 2.18507 factor:1 | 1 (-0.97882) | -1 | -1 |
| G: -5684.20830 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.51973 HOMO: -6.18243 LUMO: 2.01636 factor:1 | 1 (-0.94573) | -1 | -1 |
| G: -5684.20830 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.52746 HOMO: -6.99877 LUMO: 2.14970 factor:1 | 1 (-0.95346) | 1 | 1 |
| G: -5684.20830 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.60082 HOMO: -6.72665 LUMO: 2.07079 factor:1 | 1 (-1.02682) | 1 | 1 |
| G: -5684.20830 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.45815 HOMO: -6.36202 LUMO: 2.17419 factor:1 | 1 (-0.88415) | -1 | -1 |
| G: -5684.20830 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.57709 HOMO: -6.78652 LUMO: 2.05718 factor:1 | 1 (-1.00309) | 1 | -1 |
| G: -5684.20830 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.85917 HOMO: -6.87360 LUMO: 2.34290 factor:1 | 1 (-1.28517) | 1 | 1 |
| G: -5684.20830 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.41527 HOMO: -6.62053 LUMO: 1.89391 factor:1 | 1 (-0.84127) | 1 | 1 |
| G: -5684.20830 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.51624 HOMO: -6.58788 LUMO: 1.83133 factor:1 | 1 (-1.94224) | 1 | 1 |
| G: -5684.20830 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.99490 HOMO: -7.08584 LUMO: 1.91568 factor:1 | 1 (-1.42090) | 1 | 1 |
| G: -5684.20830 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.84017 HOMO: -6.56883 LUMO: 1.81228 factor:1 | 1 (-1.26617) | 1 | 1 |
| G: -5684.20830 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.80621 HOMO: -6.66135 LUMO: 1.92384 factor:1 | 1 (-1.23221) | 1 | 1 |
| G: -5684.20830 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.05816 HOMO: -6.64502 LUMO: 2.15786 factor:1 | 1 (-1.48416) | 1 | 1 |
| G: -5684.20830 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.99258 HOMO: -6.71305 LUMO: 1.91840 factor:1 | 1 (-1.41858) | 1 | 1 |
| G: -5684.20830 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.33169 HOMO: -6.44094 LUMO: 1.74425 factor:1 | 1 (-1.75769) | -1 | -1 |
| G: -5684.20830 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.61042 HOMO: -6.51985 LUMO: 1.84221 factor:1 | 1 (-2.03642) | -1 | -1 |
| G: -5684.20830 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.87655 HOMO: -6.63414 LUMO: -0.24762 factor:1 | 1 (-1.30255) | -1 | -1 |
| G: -5684.20830 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.98349 HOMO: -6.60420 LUMO: -0.22585 factor:1 | 1 (-1.40950) | -1 | -1 |
| G: -5684.20830 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.56895 HOMO: -7.19741 LUMO: 0.58232 factor:1 | 1 (-1.99495) | -1 | -1 |
| G: -5684.20830 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.74714 HOMO: -6.77019 LUMO: -0.56872 factor:1 | 1 (-1.17314) | -1 | -1 |
| G: -5684.20830 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.60531 HOMO: -7.46136 LUMO: 0.28844 factor:1 | 1 (-1.03131) | -1 | -1 |
| G: -5684.20830 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.62964 HOMO: -6.60420 LUMO: -0.54151 factor:1 | 1 (-1.05564) | -1 | -1 |
| G: -5684.20830 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.67290 HOMO: -6.53890 LUMO: -0.46531 factor:1 | 1 (-1.09890) | -1 | -1 |
| G: -5684.20830 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.16203 HOMO: -6.81645 LUMO: -0.57144 factor:1 | 1 (-1.58803) | -1 | -1 |
| G: -5684.20830 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.55138 HOMO: -7.48041 LUMO: 0.28572 factor:1 | 1 (-0.97738) | -1 | -1 |
| G: -5684.20830 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.61617 HOMO: -6.75659 LUMO: -0.45715 factor:1 | 1 (-1.04217) | -1 | -1 |
| G: -5684.20830 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.69397 HOMO: -6.66135 LUMO: -0.41906 factor:1 | 1 (-1.11997) | -1 | -1 |
| G: -5684.20830 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.34340 HOMO: -6.55794 LUMO: -0.27483 factor:1 | 1 (-0.76940) | -1 | -1 |
| G: -5684.20830 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11951.13162 HOMO: -7.07496 LUMO: -0.63403 factor:1 | 1 (-2.55763) | -1 | -1 |
| G: -5684.20830 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.15435 HOMO: -7.12394 LUMO: 0.53334 factor:1 | 1 (-1.58036) | -1 | -1 |
| G: -5684.20830 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11951.12093 HOMO: -6.53617 LUMO: -0.25579 factor:1 | 1 (-2.54693) | -1 | -1 |
| G: -5684.20830 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.82768 HOMO: -6.50896 LUMO: -0.25034 factor:1 | 1 (-1.25368) | -1 | -1 |
| G: -5684.20830 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.78371 HOMO: -7.17564 LUMO: -0.68573 factor:1 | 1 (-1.20971) | -1 | -1 |
| G: -5684.20830 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.89868 HOMO: -6.53617 LUMO: -0.30749 factor:1 | 1 (-1.32468) | -1 | -1 |
| G: -5684.20830 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.99043 HOMO: -6.55522 LUMO: -0.30749 factor:1 | 1 (-1.41643) | -1 | -1 |
| G: -5684.20830 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.90281 HOMO: -7.05591 LUMO: -0.71022 factor:1 | 1 (-1.32881) | -1 | -1 |
| G: -5684.20830 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.10377 HOMO: -7.17564 LUMO: -0.69933 factor:1 | 1 (-1.52977) | -1 | -1 |
| G: -5684.20830 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.37550 HOMO: -6.78380 LUMO: -0.67756 factor:1 | 1 (-1.80150) | -1 | -1 |
| G: -5684.20830 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.52854 HOMO: -6.62325 LUMO: 2.02725 factor:1 | 1 (-1.95454) | 1 | 1 |
| G: -5684.20830 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.92997 HOMO: -6.63414 LUMO: 1.91296 factor:1 | 1 (-1.35597) | 1 | -1 |
| G: -5684.20830 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.96336 HOMO: -6.83278 LUMO: 1.65717 factor:1 | 1 (-1.38936) | 1 | 1 |
| G: -5684.20830 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.90107 HOMO: -6.66407 LUMO: 1.95650 factor:1 | 1 (-1.32707) | 1 | 1 |
| G: -5684.20830 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.61617 HOMO: -6.61237 LUMO: 2.11432 factor:1 | 1 (-1.04217) | 1 | 1 |
| G: -5684.20830 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.70637 HOMO: -6.62053 LUMO: 2.09256 factor:1 | 1 (-1.13237) | 1 | -1 |
| G: -5684.20830 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.26793 HOMO: -6.78652 LUMO: 2.13609 factor:1 | 1 (-1.69394) | 1 | 1 |
| G: -5684.20830 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.59034 HOMO: -6.94707 LUMO: 1.81772 factor:1 | 1 (-1.01635) | 1 | 1 |
| G: -5684.20830 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.52125 HOMO: -6.85183 LUMO: 2.12793 factor:1 | 1 (-0.94726) | 1 | 1 |
| G: -5684.20830 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.65181 HOMO: -6.81101 LUMO: 1.83949 factor:1 | 1 (-1.07782) | 1 | 1 |
| G: -5684.20830 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.79633 HOMO: -6.98788 LUMO: 2.16058 factor:1 | 1 (-1.22234) | 1 | 1 |
| G: -5684.20830 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.74648 HOMO: -6.62869 LUMO: 2.00820 factor:1 | 1 (-1.17248) | 1 | 1 |
| G: -5684.20830 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.98216 HOMO: -6.34025 LUMO: 2.25855 factor:1 | 1 (-1.40816) | -1 | -1 |
| G: -5684.20830 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.04638 HOMO: -6.01372 LUMO: 2.01636 factor:1 | 1 (-1.47238) | -1 | -1 |
| G: -5684.20830 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.79884 HOMO: -6.89264 LUMO: 2.27487 factor:1 | 1 (-1.22484) | 1 | 1 |
| G: -5684.20830 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.88836 HOMO: -6.53073 LUMO: 2.20684 factor:1 | 1 (-1.31436) | -1 | -1 |
| G: -5684.20830 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.74934 HOMO: -6.83278 LUMO: 1.53744 factor:1 | 1 (-1.17534) | -1 | -1 |
| G: -5684.20830 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.90698 HOMO: -6.41917 LUMO: 1.82316 factor:1 | 1 (-1.33298) | -1 | -1 |
| G: -5684.20830 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.49742 HOMO: -6.56339 LUMO: 1.63813 factor:1 | 1 (-0.92342) | -1 | -1 |
| G: -5684.20830 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.59062 HOMO: -6.88992 LUMO: 1.65173 factor:1 | 1 (-1.01662) | 1 | 1 |
| G: -5684.20830 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.38838 HOMO: -6.63141 LUMO: 1.92112 factor:1 | 1 (-0.81438) | 1 | 1 |
| G: -5684.20830 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.41796 HOMO: -6.83822 LUMO: 1.88847 factor:1 | 1 (-0.84396) | 1 | 1 |
| G: -5684.20830 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.59459 HOMO: -6.84638 LUMO: 1.90480 factor:1 | 1 (-1.02059) | 1 | 1 |
| G: -5684.20830 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.02281 HOMO: -6.82462 LUMO: 1.70888 factor:1 | 1 (-1.44882) | 1 | 1 |
| G: -5684.20830 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.99680 HOMO: -6.82734 LUMO: 2.12521 factor:1 | 1 (-1.42280) | 1 | 1 |
| G: -5684.20830 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.90981 HOMO: -6.94435 LUMO: 1.87214 factor:1 | 1 (-1.33581) | 1 | 1 |
| G: -5684.20830 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.81380 HOMO: -6.98516 LUMO: 2.51433 factor:1 | 1 (-1.23981) | 1 | 1 |
| G: -5684.20830 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.45875 HOMO: -6.74026 LUMO: 2.15514 factor:1 | 1 (-0.88475) | 1 | 1 |
| G: -5684.20830 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.33159 HOMO: -6.93618 LUMO: 2.54426 factor:1 | 1 (-0.75759) | 1 | 1 |
| G: -5684.20830 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.05994 HOMO: -6.28583 LUMO: 2.53610 factor:1 | 1 (-0.48594) | -1 | -1 |
| G: -5684.20830 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.07874 HOMO: -6.56883 LUMO: 1.94834 factor:1 | 1 (-0.50474) | 1 | 1 |
| G: -5684.20830 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.40751 HOMO: -7.08584 LUMO: 1.99187 factor:1 | 1 (-0.83351) | 1 | 1 |
| G: -5684.20830 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.42672 HOMO: -6.19059 LUMO: 1.99732 factor:1 | 1 (-0.85272) | -1 | -1 |
| G: -5684.20830 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.12002 HOMO: -6.78108 LUMO: 2.03813 factor:1 | 1 (-0.54602) | 1 | 1 |
| G: -5684.20830 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.59848 HOMO: -6.82189 LUMO: 1.77418 factor:1 | 1 (-1.02448) | 1 | 1 |
| G: -5684.20830 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.38747 HOMO: -6.45454 LUMO: 1.78779 factor:1 | 1 (-1.81348) | -1 | -1 |
| G: -5684.20830 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.74915 HOMO: -6.84366 LUMO: 1.77690 factor:1 | 1 (-1.17515) | 1 | 1 |
| G: -5684.20830 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.81002 HOMO: -6.74026 LUMO: 1.67622 factor:1 | 1 (-1.23602) | 1 | 1 |
| G: -5684.20830 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.98126 HOMO: -6.76475 LUMO: 2.40277 factor:1 | 1 (-1.40726) | 1 | 1 |
| G: -5684.20830 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.01174 HOMO: -6.65863 LUMO: 1.86670 factor:1 | 1 (-1.43774) | 1 | 1 |
| G: -5684.20830 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.56413 HOMO: -6.50080 LUMO: 1.93201 factor:1 | 1 (-1.99013) | -1 | -1 |
| G: -5684.20830 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.81427 HOMO: -6.34842 LUMO: 1.70888 factor:1 | 1 (-1.24027) | -1 | -1 |
| G: -5684.20830 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.79163 HOMO: -6.60692 LUMO: 2.20140 factor:1 | 1 (-1.21763) | 1 | 1 |
| G: -5684.20830 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.91098 HOMO: -6.74026 LUMO: 2.14970 factor:1 | 1 (-1.33698) | 1 | 1 |
| G: -5684.20830 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.56881 HOMO: -6.63686 LUMO: 2.17419 factor:1 | 1 (-1.99481) | 1 | 1 |
| G: -5684.20830 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.69190 HOMO: -6.81917 LUMO: 2.10072 factor:1 | 1 (-1.11790) | 1 | -1 |
| G: -5684.20830 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.69026 HOMO: -6.92802 LUMO: 2.04358 factor:1 | 1 (-1.11627) | 1 | 1 |
| G: -5684.20830 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.70335 HOMO: -6.56067 LUMO: -0.47620 factor:1 | 1 (-1.12935) | -1 | -1 |
| G: -5684.20830 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.73489 HOMO: -6.56611 LUMO: -0.77008 factor:1 | 1 (-1.16089) | -1 | -1 |
| G: -5684.20830 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.60501 HOMO: -6.78380 LUMO: -0.64763 factor:1 | 1 (-1.03101) | -1 | -1 |
| G: -5684.20830 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.76798 HOMO: -6.51985 LUMO: -0.24490 factor:1 | 1 (-1.19398) | -1 | -1 |
| G: -5684.20830 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.35264 HOMO: -6.52529 LUMO: -0.27483 factor:1 | 1 (-1.77865) | -1 | -1 |
| G: -5684.20830 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.52188 HOMO: -7.10489 LUMO: -0.62586 factor:1 | 1 (-0.94788) | -1 | -1 |
| G: -5684.20830 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.46817 HOMO: -7.18108 LUMO: 0.48980 factor:1 | 1 (-0.89417) | -1 | -1 |
| G: -5684.20830 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.88887 HOMO: -7.14299 LUMO: -0.63947 factor:1 | 1 (-2.31487) | -1 | -1 |
| G: -5684.20830 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.71250 HOMO: -6.70761 LUMO: -0.54423 factor:1 | 1 (-1.13850) | -1 | -1 |
| G: -5684.20830 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.44789 HOMO: -7.32258 LUMO: -1.03675 factor:1 | 1 (-0.87389) | -1 | -1 |
| G: -5684.20830 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.57165 HOMO: -6.65046 LUMO: -0.41361 factor:1 | 1 (-0.99765) | -1 | -1 |
| G: -5684.20830 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.35273 HOMO: -6.76475 LUMO: -0.60137 factor:1 | 1 (-0.77874) | -1 | -1 |
| G: -5684.20830 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.09438 HOMO: -6.77836 LUMO: -0.54423 factor:1 | 1 (-1.52038) | -1 | -1 |
| G: -5684.20830 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.97051 HOMO: -7.52395 LUMO: 0.26395 factor:1 | 1 (-1.39652) | -1 | -1 |
| G: -5684.20830 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.08012 HOMO: -6.93890 LUMO: -0.72382 factor:1 | 1 (-1.50612) | -1 | -1 |
| G: -5684.20830 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.97653 HOMO: -6.72938 LUMO: -0.47348 factor:1 | 1 (-1.40253) | -1 | -1 |
| G: -5684.20830 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.38746 HOMO: -6.66951 LUMO: -0.40817 factor:1 | 1 (-0.81346) | -1 | -1 |
| G: -5684.20830 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.18767 HOMO: -6.60420 LUMO: -0.19320 factor:1 | 1 (-0.61367) | -1 | -1 |
| G: -5684.20830 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.31235 HOMO: -6.67495 LUMO: -0.27211 factor:1 | 1 (-0.73835) | -1 | -1 |
| G: -5684.20830 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.20865 HOMO: -7.23823 LUMO: -0.62858 factor:1 | 1 (-0.63465) | -1 | -1 |
| G: -5684.20830 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.50980 HOMO: -7.27088 LUMO: 0.53334 factor:1 | 1 (-0.93580) | -1 | -1 |
| G: -5684.20830 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.18944 HOMO: -7.20013 LUMO: 0.59049 factor:1 | 1 (-0.61544) | -1 | -1 |
| G: -5684.20830 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.43859 HOMO: -6.60148 LUMO: -0.20953 factor:1 | 1 (-0.86459) | -1 | -1 |
| G: -5684.20830 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.73473 HOMO: -6.69400 LUMO: -0.51974 factor:1 | 1 (-1.16073) | -1 | -1 |
| G: -5684.20830 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.78480 HOMO: -7.40422 LUMO: -0.98777 factor:1 | 1 (-1.21080) | -1 | -1 |
| G: -5684.20830 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.53644 HOMO: -6.88176 LUMO: -0.71022 factor:1 | 1 (-0.96244) | -1 | -1 |
| G: -5684.20830 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.14848 HOMO: -6.86271 LUMO: -0.59321 factor:1 | 1 (-1.57448) | -1 | -1 |
| G: -5684.20830 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.11435 HOMO: -6.73754 LUMO: -0.55239 factor:1 | 1 (-1.54035) | -1 | -1 |
| G: -5684.20830 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.08434 HOMO: -6.71033 LUMO: 1.57010 factor:1 | 1 (-1.51034) | -1 | -1 |
| G: -5684.20830 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.91530 HOMO: -6.69672 LUMO: 1.68711 factor:1 | 1 (-1.34130) | 1 | 1 |
| G: -5684.20830 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.48558 HOMO: -6.67495 LUMO: 2.03813 factor:1 | 1 (-0.91158) | 1 | 1 |
| G: -5684.20830 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.27472 HOMO: -6.54434 LUMO: 1.83677 factor:1 | 1 (-0.70072) | -1 | -1 |
| G: -5684.20830 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.43393 HOMO: -6.57155 LUMO: 1.77146 factor:1 | 1 (-0.85993) | 1 | 1 |
| G: -5684.20830 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.33399 HOMO: -6.76747 LUMO: 1.87759 factor:1 | 1 (-0.75999) | 1 | 1 |
| G: -5684.20830 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.70896 HOMO: -6.58243 LUMO: 1.61364 factor:1 | 1 (-1.13496) | 1 | 1 |
| G: -5684.20830 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.77853 HOMO: -6.61781 LUMO: 2.13881 factor:1 | 1 (-2.20453) | 1 | 1 |
| G: -5684.20830 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.66338 HOMO: -6.62597 LUMO: 2.00276 factor:1 | 1 (-1.08938) | 1 | 1 |
| G: -5684.20830 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.70450 HOMO: -7.01237 LUMO: 1.95922 factor:1 | 1 (-1.13050) | 1 | 1 |
| G: -5684.20830 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.80687 HOMO: -7.03959 LUMO: 2.16875 factor:1 | 1 (-1.23287) | 1 | 1 |
| G: -5684.20830 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.83870 HOMO: -6.83278 LUMO: 1.91296 factor:1 | 1 (-1.26470) | 1 | 1 |
| G: -5684.20830 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.86687 HOMO: -6.40012 LUMO: 1.95650 factor:1 | 1 (-1.29287) | -1 | -1 |
| G: -5684.20830 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.04387 HOMO: -6.50080 LUMO: 1.73337 factor:1 | -1 (0.53013) | -1 | -1 |
| G: -5684.20830 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.86483 HOMO: -6.95795 LUMO: 2.28848 factor:1 | 1 (-1.29083) | 1 | 1 |
| G: -5684.20830 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.68711 HOMO: -6.63686 LUMO: 2.20140 factor:1 | 1 (-1.11311) | 1 | -1 |
| G: -5684.20830 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.71089 HOMO: -6.57427 LUMO: 1.87214 factor:1 | 1 (-1.13689) | 1 | -1 |
| G: -5684.20830 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.66387 HOMO: -6.38379 LUMO: 2.32113 factor:1 | 1 (-1.08987) | -1 | -1 |
| G: -5684.20830 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.73163 HOMO: -6.63958 LUMO: 2.04902 factor:1 | 1 (-1.15763) | 1 | 1 |
| G: -5684.20830 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.45002 HOMO: -6.70216 LUMO: 1.93201 factor:1 | 1 (-0.87602) | 1 | 1 |
| G: -5684.20830 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.55342 HOMO: -6.80557 LUMO: 2.23678 factor:1 | 1 (-0.97942) | 1 | 1 |
| G: -5684.20830 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.70618 HOMO: -6.72938 LUMO: 2.28304 factor:1 | 1 (-1.13218) | 1 | 1 |
| G: -5684.20830 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.22593 HOMO: -6.56067 LUMO: 1.66806 factor:1 | 1 (-0.65193) | -1 | -1 |
| G: -5684.20830 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.00620 HOMO: -6.95523 LUMO: 2.33474 factor:1 | 1 (-0.43220) | 1 | 1 |
| G: -5684.20830 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.38226 HOMO: -6.59876 LUMO: 2.30480 factor:1 | 1 (-0.80826) | 1 | 1 |
| G: -5684.20830 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.06503 HOMO: -6.87360 LUMO: 1.75786 factor:1 | 1 (-0.49103) | 1 | 1 |
| G: -5684.20830 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.56980 HOMO: -7.06408 LUMO: 1.99187 factor:1 | 1 (-0.99580) | 1 | 1 |
| G: -5684.20830 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.89007 HOMO: -6.95795 LUMO: 1.88847 factor:1 | 1 (-2.31607) | 1 | 1 |
| G: -5684.20830 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.86156 HOMO: -6.85455 LUMO: 1.63813 factor:1 | 1 (-1.28756) | 1 | 1 |
| G: -5684.20830 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.70319 HOMO: -7.09129 LUMO: 2.31569 factor:1 | 1 (-1.12919) | 1 | 1 |
| G: -5684.20830 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.79484 HOMO: -6.91441 LUMO: 1.68983 factor:1 | 1 (-1.22084) | 1 | 1 |
| G: -5684.20830 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.96746 HOMO: -6.89809 LUMO: 2.23678 factor:1 | 1 (-2.39346) | 1 | 1 |
| G: -5684.20830 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.74205 HOMO: -6.78652 LUMO: 1.98371 factor:1 | 1 (-1.16805) | 1 | -1 |
| G: -5684.20830 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.77013 HOMO: -6.94707 LUMO: 2.23678 factor:1 | 1 (-1.19613) | 1 | 1 |
| G: -5684.20830 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.06886 HOMO: -7.07224 LUMO: 2.13337 factor:1 | 1 (-1.49486) | 1 | 1 |
| G: -5684.20830 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.23359 HOMO: -6.94979 LUMO: 2.28031 factor:1 | 1 (-1.65960) | 1 | 1 |
| G: -5684.20830 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.42509 HOMO: -6.60965 LUMO: 2.20412 factor:1 | 1 (-0.85109) | 1 | 1 |
| G: -5684.20830 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.99201 HOMO: -6.87360 LUMO: 2.40277 factor:1 | 1 (-1.41801) | 1 | -1 |
| G: -5684.20830 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.44245 HOMO: -6.92802 LUMO: 1.89663 factor:1 | 1 (-0.86845) | 1 | -1 |
| G: -5684.20830 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.57113 HOMO: -6.88448 LUMO: 2.02725 factor:1 | 1 (-0.99713) | 1 | 1 |
| G: -5684.20830 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.32528 HOMO: -6.69128 LUMO: 1.55105 factor:1 | 1 (-0.75128) | -1 | -1 |
| G: -5684.20830 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.75454 HOMO: -6.54978 LUMO: 1.93201 factor:1 | 1 (-1.18054) | -1 | -1 |
| G: -5684.20830 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.27330 HOMO: -6.19331 LUMO: 1.46941 factor:1 | 1 (-0.69931) | -1 | -1 |
| G: -5684.20830 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.51608 HOMO: -6.55794 LUMO: 1.89663 factor:1 | 1 (-0.94209) | -1 | -1 |
| G: -5684.20830 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.57189 HOMO: -6.07630 LUMO: 1.94289 factor:1 | 1 (-0.99790) | -1 | -1 |
| G: -5684.20830 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.76112 HOMO: -7.46408 LUMO: 0.31565 factor:1 | 1 (-1.18712) | -1 | -1 |
| G: -5684.20830 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.08872 HOMO: -6.63958 LUMO: -0.61770 factor:1 | 1 (-1.51472) | -1 | -1 |
| G: -5684.20830 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.43165 HOMO: -6.81101 LUMO: -0.57960 factor:1 | 1 (-0.85765) | -1 | -1 |
| G: -5684.20830 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.07563 HOMO: -6.74298 LUMO: -0.57960 factor:1 | 1 (-1.50163) | -1 | -1 |
| G: -5684.20830 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.41480 HOMO: -6.63686 LUMO: -0.42994 factor:1 | 1 (-0.84080) | -1 | -1 |
| G: -5684.20830 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.61652 HOMO: -6.60965 LUMO: -0.41089 factor:1 | 1 (-1.04252) | -1 | -1 |
| G: -5684.20830 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.55462 HOMO: -6.60692 LUMO: -0.80274 factor:1 | 1 (-0.98062) | -1 | -1 |
| G: -5684.20830 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.82001 HOMO: -6.58788 LUMO: -0.78097 factor:1 | 1 (-1.24601) | -1 | -1 |
| G: -5684.20830 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.40090 HOMO: -6.67767 LUMO: -0.48436 factor:1 | 1 (-0.82690) | -1 | -1 |
| G: -5684.20830 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.64629 HOMO: -6.63141 LUMO: -0.40545 factor:1 | 1 (-1.07229) | -1 | -1 |
| G: -5684.20830 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.66455 HOMO: -6.62053 LUMO: -0.83811 factor:1 | 1 (-1.09055) | -1 | -1 |
| G: -5684.20830 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.84526 HOMO: -6.59604 LUMO: -0.35375 factor:1 | 1 (-1.27126) | -1 | -1 |
| G: -5684.20830 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.99552 HOMO: -6.34297 LUMO: -0.39729 factor:1 | 1 (-1.42152) | -1 | -1 |
| G: -5684.20830 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.14543 HOMO: -6.67223 LUMO: 1.97827 factor:1 | 1 (-1.57143) | 1 | 1 |
| G: -5684.20830 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.30257 HOMO: -6.40012 LUMO: 1.89935 factor:1 | 1 (-1.72858) | -1 | -1 |
| G: -5684.20830 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.50468 HOMO: -6.74842 LUMO: 1.97283 factor:1 | 1 (-0.93068) | 1 | -1 |
| G: -5684.20830 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.52602 HOMO: -6.76747 LUMO: 2.17147 factor:1 | 1 (-0.95202) | 1 | 1 |
| G: -5684.20830 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.69383 HOMO: -6.72121 LUMO: 1.55649 factor:1 | 1 (-1.11983) | -1 | -1 |
| G: -5684.20830 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.14644 HOMO: -6.97700 LUMO: 2.04085 factor:1 | 1 (-1.57244) | 1 | 1 |
| G: -5684.20830 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.01543 HOMO: -7.06680 LUMO: 2.04085 factor:1 | -1 (0.55857) | 1 | -1 |
| G: -5684.20830 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.22941 HOMO: -7.09673 LUMO: 2.35106 factor:1 | 1 (-0.65541) | 1 | 1 |
| G: -5684.20830 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.49848 HOMO: -6.83006 LUMO: 2.14970 factor:1 | 1 (-0.92448) | 1 | 1 |
| G: -5684.20830 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.78425 HOMO: -6.72665 LUMO: 2.20140 factor:1 | 1 (-1.21025) | 1 | -1 |
| G: -5684.20830 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.53745 HOMO: -6.77291 LUMO: 2.34562 factor:1 | 1 (-0.96345) | 1 | -1 |
| G: -5684.20830 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.03949 HOMO: -6.73754 LUMO: 2.00276 factor:1 | -1 (1.53450) | 1 | -1 |
| G: -5684.20830 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.72847 HOMO: -7.04231 LUMO: 1.92112 factor:1 | 1 (-1.15447) | 1 | -1 |
| G: -5684.20830 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.20249 HOMO: -6.83822 LUMO: 1.72248 factor:1 | 1 (-1.62849) | 1 | 1 |
| G: -5684.20830 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.18089 HOMO: -6.57971 LUMO: 2.16603 factor:1 | 1 (-1.60689) | 1 | -1 |
| G: -5684.20830 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.38913 HOMO: -6.80013 LUMO: 1.88575 factor:1 | 1 (-1.81514) | 1 | 1 |
| G: -5684.20830 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.65459 HOMO: -6.93618 LUMO: 2.18235 factor:1 | 1 (-1.08059) | 1 | 1 |
| G: -5684.20830 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.66047 HOMO: -6.54706 LUMO: 1.91024 factor:1 | 1 (-1.08647) | -1 | -1 |
| G: -5684.20830 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.09386 HOMO: -7.06952 LUMO: 2.18507 factor:1 | 1 (-1.51986) | 1 | 1 |
| G: -5684.20830 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.27876 HOMO: -7.05047 LUMO: 1.82044 factor:1 | 1 (-1.70477) | 1 | 1 |
| G: -5684.20830 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.96981 HOMO: -6.87632 LUMO: 1.92657 factor:1 | 1 (-1.39581) | 1 | 1 |
| G: -5684.20830 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.43045 HOMO: -6.58788 LUMO: 1.91568 factor:1 | 1 (-0.85645) | 1 | -1 |
| G: -5684.20830 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.60384 HOMO: -7.17292 LUMO: 1.90752 factor:1 | 1 (-1.02984) | 1 | 1 |
| G: -5684.20830 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.86991 HOMO: -6.93890 LUMO: 1.80684 factor:1 | 1 (-1.29592) | 1 | 1 |
| G: -5684.20830 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.85712 HOMO: -7.10761 LUMO: 2.20956 factor:1 | 1 (-1.28313) | 1 | 1 |
| G: -5684.20830 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.70931 HOMO: -6.85727 LUMO: 2.13609 factor:1 | 1 (-1.13531) | 1 | -1 |
| G: -5684.20830 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.42019 HOMO: -6.64502 LUMO: 1.38506 factor:1 | 1 (-0.84619) | -1 | -1 |
| G: -5684.20830 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.81987 HOMO: -6.87360 LUMO: 1.15648 factor:1 | 1 (-1.24587) | -1 | -1 |
| G: -5684.20830 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.91448 HOMO: -6.67223 LUMO: 2.07351 factor:1 | 1 (-2.34048) | 1 | 1 |
| G: -5684.20830 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.86357 HOMO: -6.29671 LUMO: 2.43270 factor:1 | 1 (-1.28957) | -1 | -1 |
| G: -5684.20830 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.84762 HOMO: -6.90897 LUMO: 2.28848 factor:1 | 1 (-2.27362) | 1 | 1 |
| G: -5684.20830 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.16399 HOMO: -7.04231 LUMO: 1.70071 factor:1 | 1 (-1.58999) | 1 | 1 |
| G: -5684.20830 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.26440 HOMO: -6.69944 LUMO: 1.94834 factor:1 | 1 (-1.69040) | 1 | 1 |
| G: -5684.20830 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.70009 HOMO: -6.56067 LUMO: 2.20956 factor:1 | 1 (-1.12609) | -1 | -1 |
| G: -5684.20830 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.14325 HOMO: -6.65046 LUMO: 2.06807 factor:1 | 1 (-1.56925) | 1 | -1 |
| G: -5684.20830 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.53750 HOMO: -7.08584 LUMO: 1.98915 factor:1 | 1 (-0.96350) | 1 | 1 |
| G: -5684.20830 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.92344 HOMO: -6.69400 LUMO: 2.09256 factor:1 | 1 (-1.34944) | 1 | 1 |
| G: -5684.20830 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.55750 HOMO: -6.62869 LUMO: 2.16331 factor:1 | 1 (-0.98350) | 1 | 1 |
| G: -5684.20830 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.89005 HOMO: -6.85183 LUMO: 2.16058 factor:1 | 1 (-1.31605) | 1 | 1 |
| G: -5684.20830 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.35940 HOMO: -6.54706 LUMO: 1.92384 factor:1 | 1 (-0.78540) | -1 | -1 |
| G: -5684.20830 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.61538 HOMO: -6.84366 LUMO: 2.48984 factor:1 | 1 (-1.04138) | 1 | 1 |
| G: -5684.20830 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.10750 HOMO: -6.77291 LUMO: 2.46263 factor:1 | 1 (-1.53350) | 1 | 1 |
| G: -5684.20830 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.78126 HOMO: -7.01782 LUMO: 2.31025 factor:1 | 1 (-1.20726) | 1 | 1 |
| G: -5684.20830 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.59127 HOMO: -6.94707 LUMO: 2.29664 factor:1 | 1 (-1.01727) | 1 | 1 |
| G: -5684.20830 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.33260 HOMO: -6.64230 LUMO: 1.97283 factor:1 | 1 (-0.75860) | 1 | 1 |
| G: -5684.20830 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.36732 HOMO: -6.47359 LUMO: 2.20412 factor:1 | 1 (-0.79332) | -1 | -1 |
| G: -5684.20830 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.44229 HOMO: -6.90625 LUMO: 1.92384 factor:1 | 1 (-0.86829) | 1 | 1 |
| G: -5684.20830 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.15314 HOMO: -7.17020 LUMO: 2.06807 factor:1 | 1 (-0.57914) | 1 | 1 |
| G: -5684.20830 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.46980 HOMO: -6.65046 LUMO: 2.20956 factor:1 | 1 (-0.89580) | 1 | -1 |
| G: -5684.20830 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.62708 HOMO: -7.07496 LUMO: 1.82861 factor:1 | 1 (-1.05308) | 1 | 1 |
| G: -5684.20830 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.85976 HOMO: -6.83006 LUMO: 2.14970 factor:1 | 1 (-1.28577) | 1 | -1 |
| G: -5684.20830 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.52085 HOMO: -6.92802 LUMO: 1.99187 factor:1 | 1 (-0.94685) | 1 | 1 |
| G: -5684.20830 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.62898 HOMO: -6.69672 LUMO: 2.36739 factor:1 | 1 (-1.05499) | 1 | -1 |
| G: -5684.20830 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.67434 HOMO: -7.13755 LUMO: 2.00276 factor:1 | 1 (-2.10034) | 1 | 1 |
| G: -5684.20830 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.46104 HOMO: -6.92530 LUMO: 2.25582 factor:1 | 1 (-0.88704) | 1 | 1 |
| G: -5684.20830 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.76058 HOMO: -6.77564 LUMO: 1.97827 factor:1 | 1 (-1.18658) | 1 | 1 |
| G: -5684.20830 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.99400 HOMO: -6.87904 LUMO: 1.60003 factor:1 | 1 (-1.42000) | 1 | 1 |
| G: -5684.20830 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.67666 HOMO: -6.62869 LUMO: 1.90480 factor:1 | 1 (-1.10266) | 1 | 1 |
| G: -5684.20830 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.71742 HOMO: -6.71033 LUMO: 1.54833 factor:1 | 1 (-1.14342) | -1 | -1 |
| G: -5684.20830 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.64286 HOMO: -6.74298 LUMO: 1.47486 factor:1 | 1 (-1.06886) | -1 | -1 |
| G: -5684.20830 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.70882 HOMO: -6.77019 LUMO: 1.90480 factor:1 | 1 (-1.13482) | 1 | 1 |
| G: -5684.20830 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.82790 HOMO: -6.70489 LUMO: 1.99459 factor:1 | 1 (-1.25390) | 1 | 1 |
| G: -5684.20830 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.88232 HOMO: -6.73482 LUMO: 2.08711 factor:1 | 1 (-1.30832) | 1 | 1 |
| G: -5684.20830 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.38384 HOMO: -6.46543 LUMO: 1.73881 factor:1 | 1 (-0.80984) | -1 | -1 |
| G: -5684.20830 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.54934 HOMO: -6.96067 LUMO: 2.26127 factor:1 | 1 (-0.97534) | 1 | 1 |
| G: -5684.20830 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.78697 HOMO: -6.67767 LUMO: 2.10616 factor:1 | 1 (-1.21297) | 1 | 1 |
| G: -5684.20830 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.69402 HOMO: -6.28855 LUMO: 2.35923 factor:1 | 1 (-1.12002) | -1 | -1 |
| G: -5684.20830 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.60896 HOMO: -6.80285 LUMO: 1.62724 factor:1 | 1 (-1.03496) | 1 | 1 |
| G: -5684.20830 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.78569 HOMO: -6.85455 LUMO: 2.23133 factor:1 | 1 (-1.21170) | 1 | 1 |
| G: -5684.20830 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.22256 HOMO: -6.51713 LUMO: 2.33474 factor:1 | 1 (-0.64856) | -1 | -1 |
| G: -5684.20830 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.46898 HOMO: -6.88176 LUMO: 2.15242 factor:1 | 1 (-0.89498) | 1 | 1 |
| G: -5684.20830 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.17319 HOMO: -6.54434 LUMO: 2.32113 factor:1 | 1 (-0.59919) | -1 | -1 |
| G: -5684.20830 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.98356 HOMO: -6.62597 LUMO: 2.24222 factor:1 | 1 (-0.40956) | 1 | 1 |
| G: -5684.20830 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.24781 HOMO: -6.74570 LUMO: 2.19868 factor:1 | 1 (-0.67381) | 1 | 1 |
| G: -5684.20830 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.97624 HOMO: -6.62869 LUMO: 1.98915 factor:1 | 1 (-0.40224) | 1 | 1 |
| G: -5684.20830 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.96029 HOMO: -6.64502 LUMO: 2.13881 factor:1 | 1 (-0.38629) | 1 | 1 |
| G: -5684.20830 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.10212 HOMO: -6.95795 LUMO: 1.82316 factor:1 | 1 (-0.52812) | 1 | 1 |
| G: -5684.20830 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.53802 HOMO: -6.77291 LUMO: 1.36329 factor:1 | 1 (-0.96402) | -1 | -1 |
| G: -5684.20830 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.30960 HOMO: -6.45726 LUMO: 1.73064 factor:1 | 1 (-0.73561) | -1 | -1 |
| G: -5684.20830 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.42046 HOMO: -6.49264 LUMO: 1.77418 factor:1 | 1 (-0.84646) | -1 | -1 |
| G: -5684.20830 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.63078 HOMO: -6.60420 LUMO: 2.20956 factor:1 | 1 (-1.05678) | 1 | 1 |
| G: -5684.20830 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.47461 HOMO: -6.56067 LUMO: 2.05718 factor:1 | 1 (-0.90062) | -1 | -1 |
| G: -5684.20830 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.58376 HOMO: -6.62597 LUMO: 1.70343 factor:1 | 1 (-1.00976) | 1 | 1 |
| G: -5684.20830 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.44550 HOMO: -6.69400 LUMO: 2.16875 factor:1 | 1 (-0.87150) | 1 | 1 |
| G: -5684.20830 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.01656 HOMO: -6.63958 LUMO: 2.11977 factor:1 | 1 (-0.44257) | 1 | 1 |
| G: -5684.20830 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.48627 HOMO: -6.92802 LUMO: 1.82044 factor:1 | -1 (0.08773) | 1 | -1 |
| G: -5684.20830 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.31108 HOMO: -6.56339 LUMO: 2.30480 factor:1 | -1 (0.26292) | -1 | -1 |
| G: -5684.20830 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.22428 HOMO: -6.63958 LUMO: 1.91024 factor:1 | -1 (0.34972) | 1 | -1 |
| G: -5684.20830 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.46896 HOMO: -6.93074 LUMO: 2.05446 factor:1 | -1 (0.10504) | 1 | 1 |
| G: -5684.20830 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.30314 HOMO: -6.61509 LUMO: 2.03813 factor:1 | -1 (0.27086) | 1 | 1 |
| G: -5684.20830 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.88976 HOMO: -6.61237 LUMO: 1.91296 factor:1 | 1 (-0.31576) | 1 | -1 |
| G: -5684.20830 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.75898 HOMO: -6.86815 LUMO: 1.95378 factor:1 | 1 (-0.18498) | 1 | 1 |
| G: -5684.20830 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.81702 HOMO: -6.63686 LUMO: 1.70888 factor:1 | 1 (-0.24302) | 1 | 1 |
| G: -5684.20830 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.70510 HOMO: -6.57971 LUMO: 2.20140 factor:1 | 1 (-0.13110) | 1 | -1 |
| G: -5684.20830 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.11290 HOMO: -6.41100 LUMO: 1.96738 factor:1 | -1 (0.46110) | -1 | -1 |
| G: -5684.20830 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11946.69244 HOMO: -6.90081 LUMO: 1.65989 factor:1 | -1 (1.88156) | 1 | 1 |
| G: -5684.20830 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.16874 HOMO: -6.68312 LUMO: 1.97827 factor:1 | -1 (0.40526) | 1 | -1 |
| G: -5684.20830 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.17135 HOMO: -6.65318 LUMO: 2.10888 factor:1 | -1 (0.40265) | 1 | -1 |
| G: -5684.20830 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.98972 HOMO: -6.62053 LUMO: 2.28848 factor:1 | -1 (0.58428) | 1 | -1 |
| G: -5684.20830 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.06836 HOMO: -6.65863 LUMO: 2.29664 factor:1 | -1 (0.50564) | 1 | -1 |
| G: -5684.20830 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.11873 HOMO: -6.63958 LUMO: 2.07623 factor:1 | -1 (0.45527) | 1 | -1 |
| G: -5684.20830 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.05981 HOMO: -6.58243 LUMO: 2.20684 factor:1 | -1 (0.51419) | 1 | 1 |
| G: -5684.20830 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.94814 HOMO: -6.59332 LUMO: 2.05174 factor:1 | -1 (0.62586) | 1 | -1 |
| G: -5684.20830 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.15775 HOMO: -6.95251 LUMO: 2.20140 factor:1 | -1 (0.41625) | 1 | 1 |
| G: -5684.20830 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.40296 HOMO: -6.84638 LUMO: 2.39732 factor:1 | -1 (1.17104) | 1 | 1 |
| G: -5684.20830 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.20733 HOMO: -6.86815 LUMO: 2.47896 factor:1 | -1 (1.36666) | 1 | 1 |
| G: -5684.20830 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.28973 HOMO: -7.00693 LUMO: 2.43270 factor:1 | -1 (1.28427) | 1 | 1 |
| G: -5684.20830 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.26668 HOMO: -6.58788 LUMO: 2.30208 factor:1 | -1 (1.30732) | 1 | 1 |
| G: -5684.20830 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11946.59799 HOMO: -6.63958 LUMO: 2.28031 factor:1 | -1 (1.97601) | 1 | 1 |
| G: -5684.20830 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.35683 HOMO: -6.74570 LUMO: 2.28304 factor:1 | -1 (1.21717) | 1 | 1 |
| G: -5684.20830 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11946.55383 HOMO: -6.78380 LUMO: 2.16331 factor:1 | -1 (2.02017) | 1 | 1 |
| G: -5684.20830 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11946.27061 HOMO: -6.52529 LUMO: 2.05718 factor:1 | -1 (2.30339) | -1 | -1 |
| G: -5684.20830 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.28559 HOMO: -6.41644 LUMO: 1.65445 factor:1 | -1 (0.28841) | -1 | -1 |
| G: -5684.20830 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.74617 HOMO: -6.34570 LUMO: 1.22451 factor:1 | -1 (0.82782) | -1 | -1 |
| G: -5684.20830 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.44179 HOMO: -6.14433 LUMO: 1.85582 factor:1 | -1 (1.13221) | -1 | -1 |
| G: -5684.20830 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.51627 HOMO: -6.62053 LUMO: 1.92112 factor:1 | -1 (1.05773) | 1 | -1 |
| G: -5684.20830 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.98073 HOMO: -6.63414 LUMO: 1.61908 factor:1 | 1 (-0.40673) | 1 | 1 |
| G: -5684.20830 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.55473 HOMO: -6.75931 LUMO: 1.87214 factor:1 | -1 (0.01927) | 1 | 1 |
| G: -5684.20830 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.15383 HOMO: -6.55794 LUMO: 1.77418 factor:1 | -1 (0.42017) | -1 | -1 |
| G: -5684.20830 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.14654 HOMO: -6.52801 LUMO: 1.82044 factor:1 | -1 (0.42746) | -1 | -1 |
| G: -5684.20830 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.51914 HOMO: -6.77564 LUMO: 1.97827 factor:1 | -1 (0.05486) | 1 | 1 |
| G: -5684.20830 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.48254 HOMO: -6.93890 LUMO: 1.81228 factor:1 | -1 (0.09146) | 1 | 1 |
| G: -5684.20830 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.08311 HOMO: -6.85455 LUMO: 1.75513 factor:1 | -1 (0.49089) | 1 | 1 |
| G: -5684.20830 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.40200 HOMO: -6.86815 LUMO: 1.64629 factor:1 | -1 (0.17200) | 1 | 1 |
| G: -5684.20830 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.69055 HOMO: -6.98516 LUMO: 1.84765 factor:1 | 1 (-0.11655) | 1 | 1 |
| G: -5684.20830 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.57716 HOMO: -6.04637 LUMO: 1.94017 factor:1 | 1 (-0.00316) | -1 | -1 |
| G: -5684.20830 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.39150 HOMO: -6.86271 LUMO: 2.11977 factor:1 | -1 (1.18250) | 1 | -1 |
| G: -5684.20830 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.30009 HOMO: -6.72938 LUMO: 2.11160 factor:1 | -1 (0.27391) | 1 | -1 |
| G: -5684.20830 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.46970 HOMO: -7.01782 LUMO: 2.13609 factor:1 | -1 (0.10430) | 1 | 1 |
| G: -5684.20830 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.64723 HOMO: -6.18515 LUMO: 2.04630 factor:1 | -1 (0.92677) | -1 | -1 |
| G: -5684.20830 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.49050 HOMO: -6.60965 LUMO: 2.17147 factor:1 | -1 (1.08350) | 1 | -1 |
| G: -5684.20830 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.60035 HOMO: -6.87360 LUMO: 2.35378 factor:1 | -1 (0.97365) | 1 | 1 |
| G: -5684.20830 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.58623 HOMO: -6.72938 LUMO: 2.20140 factor:1 | -1 (0.98777) | 1 | -1 |
| G: -5684.20830 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.91578 HOMO: -6.88448 LUMO: 2.54154 factor:1 | -1 (0.65822) | 1 | -1 |
| G: -5684.20830 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.67064 HOMO: -6.87087 LUMO: 2.16058 factor:1 | -1 (0.90336) | 1 | 1 |
| G: -5684.20830 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.05345 HOMO: -7.11306 LUMO: 2.04085 factor:1 | -1 (0.52055) | 1 | 1 |
| G: -5684.20830 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.54876 HOMO: -6.66951 LUMO: 1.68438 factor:1 | -1 (1.02524) | 1 | 1 |
| G: -5684.20830 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.56069 HOMO: -7.08312 LUMO: 2.19324 factor:1 | -1 (0.01331) | 1 | 1 |
| G: -5684.20830 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.13317 HOMO: -6.69128 LUMO: 2.13881 factor:1 | -1 (0.44082) | 1 | -1 |
| G: -5684.20830 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.19203 HOMO: -6.80285 LUMO: 2.16603 factor:1 | -1 (0.38197) | 1 | 1 |
| G: -5684.20830 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.18848 HOMO: -6.82189 LUMO: 2.46807 factor:1 | -1 (1.38552) | 1 | 1 |
| G: -5684.20830 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.33632 HOMO: -6.78652 LUMO: 2.12521 factor:1 | -1 (1.23768) | 1 | 1 |
| G: -5684.20830 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.46992 HOMO: -6.47903 LUMO: 1.70071 factor:1 | -1 (1.10407) | -1 | -1 |
| G: -5684.20830 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.29837 HOMO: -6.37019 LUMO: 1.24356 factor:1 | -1 (0.27562) | -1 | -1 |
| G: -5684.20830 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.96729 HOMO: -6.69400 LUMO: 1.67350 factor:1 | -1 (0.60671) | 1 | 1 |
| G: -5684.20830 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.26450 HOMO: -7.51851 LUMO: 0.27756 factor:1 | -1 (0.30950) | -1 | -1 |
| G: -5684.20830 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.24561 HOMO: -6.95795 LUMO: -0.72110 factor:1 | -1 (0.32839) | -1 | -1 |
| G: -5684.20830 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.02313 HOMO: -6.88720 LUMO: -0.67484 factor:1 | -1 (0.55087) | -1 | -1 |
| G: -5684.20830 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.12908 HOMO: -6.83550 LUMO: -0.57144 factor:1 | 1 (-0.55509) | -1 | -1 |
| G: -5684.20830 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.15513 HOMO: -6.80285 LUMO: -0.57144 factor:1 | 1 (-0.58113) | -1 | -1 |
| G: -5684.20830 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.22724 HOMO: -6.76475 LUMO: -0.53062 factor:1 | 1 (-0.65324) | -1 | -1 |
| G: -5684.20830 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.84530 HOMO: -6.66951 LUMO: 1.74969 factor:1 | 1 (-0.27130) | 1 | 1 |
| G: -5684.20830 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.83762 HOMO: -6.53345 LUMO: 1.89935 factor:1 | 1 (-0.26362) | -1 | -1 |
| G: -5684.20830 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.81025 HOMO: -6.65046 LUMO: 2.01364 factor:1 | 1 (-0.23625) | 1 | -1 |
| G: -5684.20830 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.66464 HOMO: -6.64230 LUMO: 2.11977 factor:1 | 1 (-0.09064) | 1 | -1 |
| G: -5684.20830 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.78842 HOMO: -6.44910 LUMO: 2.13337 factor:1 | 1 (-0.21443) | -1 | -1 |
| G: -5684.20830 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.62230 HOMO: -7.05591 LUMO: 1.98915 factor:1 | 1 (-0.04830) | 1 | -1 |
| G: -5684.20830 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.11785 HOMO: -7.02326 LUMO: 2.49256 factor:1 | -1 (0.45614) | 1 | 1 |
| G: -5684.20830 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.27485 HOMO: -6.32937 LUMO: 2.51161 factor:1 | -1 (1.29915) | -1 | -1 |
| G: -5684.20830 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.27368 HOMO: -6.96067 LUMO: 2.20140 factor:1 | -1 (1.30032) | 1 | 1 |
| G: -5684.20830 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.25068 HOMO: -6.97972 LUMO: 2.55243 factor:1 | -1 (1.32332) | 1 | 1 |
| G: -5684.20830 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.81630 HOMO: -6.72665 LUMO: 2.46535 factor:1 | -1 (0.75770) | 1 | 1 |
| G: -5684.20830 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.08923 HOMO: -6.41917 LUMO: 2.35106 factor:1 | -1 (0.48477) | -1 | -1 |
| G: -5684.20830 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.27016 HOMO: -6.75114 LUMO: 2.32929 factor:1 | -1 (0.30384) | 1 | 1 |
| G: -5684.20830 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.26112 HOMO: -6.91713 LUMO: 2.27215 factor:1 | -1 (0.31288) | 1 | 1 |
| G: -5684.20830 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.75744 HOMO: -6.54978 LUMO: 2.00276 factor:1 | -1 (0.81656) | -1 | -1 |
| G: -5684.20830 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11946.86493 HOMO: -6.62325 LUMO: 2.05990 factor:1 | -1 (1.70907) | 1 | 1 |
| G: -5684.20830 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11946.89405 HOMO: -6.86271 LUMO: 2.14970 factor:1 | -1 (1.67995) | 1 | 1 |
| G: -5684.20830 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.60201 HOMO: -6.77564 LUMO: 2.25855 factor:1 | -1 (0.97199) | 1 | -1 |
| G: -5684.20830 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.43794 HOMO: -6.71305 LUMO: 1.94561 factor:1 | -1 (0.13606) | 1 | -1 |
| G: -5684.20830 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.51235 HOMO: -6.75659 LUMO: 1.94561 factor:1 | -1 (1.06165) | 1 | -1 |
| G: -5684.20830 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.60040 HOMO: -6.94979 LUMO: 2.33474 factor:1 | -1 (0.97360) | 1 | -1 |
| G: -5684.20830 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.56530 HOMO: -6.85727 LUMO: 2.50345 factor:1 | -1 (1.00870) | 1 | -1 |
| G: -5684.20830 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.53435 HOMO: -6.87360 LUMO: 2.43270 factor:1 | -1 (0.03965) | 1 | -1 |
| G: -5684.20830 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.48412 HOMO: -6.57427 LUMO: 2.46807 factor:1 | -1 (0.08988) | 1 | -1 |
| G: -5684.20830 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.58646 HOMO: -7.16204 LUMO: 2.15242 factor:1 | 1 (-0.01246) | 1 | 1 |
| G: -5684.20830 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11946.80368 HOMO: -6.62869 LUMO: 2.11432 factor:1 | -1 (1.77032) | 1 | -1 |
| G: -5684.20830 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11946.73625 HOMO: -7.05591 LUMO: 2.26671 factor:1 | -1 (1.83775) | 1 | -1 |
| G: -5684.20830 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.39074 HOMO: -7.13483 LUMO: 1.47758 factor:1 | -1 (1.18326) | -1 | -1 |
| G: -5684.20830 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.59719 HOMO: -6.72938 LUMO: 1.57282 factor:1 | -1 (0.97681) | -1 | -1 |
| G: -5684.20830 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.61877 HOMO: -6.17426 LUMO: 1.81228 factor:1 | -1 (0.95523) | -1 | -1 |
| G: -5684.20830 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11946.80115 HOMO: -6.65318 LUMO: 1.93473 factor:1 | -1 (1.77285) | 1 | -1 |
| G: -5684.20830 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11946.78387 HOMO: -6.18515 LUMO: 2.01364 factor:1 | -1 (1.79013) | -1 | -1 |
| G: -5684.20830 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11946.80033 HOMO: -7.05591 LUMO: 2.13337 factor:1 | -1 (1.77367) | 1 | 1 |
| G: -5684.20830 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.74758 HOMO: -6.90897 LUMO: 2.29664 factor:1 | 1 (-0.17358) | 1 | -1 |
| G: -5684.20830 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11946.98230 HOMO: -7.11034 LUMO: 2.17147 factor:1 | -1 (1.59170) | 1 | 1 |
| G: -5684.20830 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11946.80847 HOMO: -6.82734 LUMO: 2.26671 factor:1 | -1 (1.76553) | 1 | 1 |
| G: -5684.20830 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11946.72229 HOMO: -6.34842 LUMO: 2.34562 factor:1 | -1 (1.85171) | -1 | -1 |
| G: -5684.20830 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11946.77105 HOMO: -6.62053 LUMO: 2.22861 factor:1 | -1 (1.80294) | 1 | -1 |
| G: -5684.20830 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11946.71160 HOMO: -6.80557 LUMO: 2.07079 factor:1 | -1 (1.86240) | 1 | -1 |
| G: -5684.20830 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.40843 HOMO: -6.60692 LUMO: 2.46263 factor:1 | -1 (1.16557) | 1 | -1 |
| G: -5684.20830 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11946.78471 HOMO: -7.02054 LUMO: 2.08711 factor:1 | -1 (1.78928) | 1 | -1 |
| G: -5684.20830 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11946.70474 HOMO: -6.78652 LUMO: 2.02453 factor:1 | -1 (1.86926) | 1 | 1 |
| G: -5684.20830 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11946.80096 HOMO: -6.51168 LUMO: 2.06534 factor:1 | -1 (1.77304) | -1 | -1 |
| G: -5684.20830 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11946.78499 HOMO: -6.50080 LUMO: 2.01636 factor:1 | -1 (1.78901) | -1 | -1 |
| G: -5684.20830 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.58544 HOMO: -6.54434 LUMO: 1.84493 factor:1 | -1 (0.98856) | -1 | -1 |
| G: -5684.20830 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.52369 HOMO: -6.47087 LUMO: 1.76330 factor:1 | -1 (1.05031) | -1 | -1 |
| G: -5684.20830 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.66265 HOMO: -6.78924 LUMO: 2.39460 factor:1 | 1 (-0.08865) | 1 | 1 |
| G: -5684.20830 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.58048 HOMO: -6.59876 LUMO: 1.84493 factor:1 | 1 (-0.00648) | 1 | 1 |
| G: -5684.20830 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.65259 HOMO: -6.41644 LUMO: 2.05174 factor:1 | 1 (-0.07859) | -1 | -1 |
| G: -5684.20830 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.78064 HOMO: -6.52257 LUMO: 2.11160 factor:1 | 1 (-0.20664) | -1 | -1 |
| G: -5684.20830 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11946.76431 HOMO: -6.90897 LUMO: 2.34018 factor:1 | -1 (1.80969) | 1 | 1 |
| G: -5684.20830 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.75762 HOMO: -6.97428 LUMO: 1.86126 factor:1 | 1 (-0.18362) | 1 | 1 |
| G: -5684.20830 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.74271 HOMO: -7.13483 LUMO: 2.14698 factor:1 | 1 (-0.16871) | 1 | -1 |
| G: -5684.20830 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.58665 HOMO: -7.16748 LUMO: 2.31841 factor:1 | 1 (-0.01265) | 1 | 1 |
| G: -5684.20830 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.70426 HOMO: -6.87087 LUMO: 2.38916 factor:1 | 1 (-0.13026) | 1 | -1 |
| G: -5684.20830 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11944.92326 HOMO: -6.93074 LUMO: 2.42181 factor:1 | -1 (3.65073) | 1 | -1 |
| G: -5684.20830 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11944.76623 HOMO: -6.90081 LUMO: 2.00276 factor:1 | -1 (3.80777) | 1 | -1 |
| G: -5684.20830 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11946.84227 HOMO: -6.99333 LUMO: 2.03541 factor:1 | -1 (1.73173) | 1 | 1 |
| G: -5684.20830 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.15816 HOMO: -6.89264 LUMO: 1.57554 factor:1 | -1 (1.41584) | -1 | -1 |
| G: -5684.20830 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.63284 HOMO: -6.48175 LUMO: 1.85854 factor:1 | -1 (0.94116) | -1 | -1 |
| G: -5684.20830 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.50647 HOMO: -6.69400 LUMO: 1.62452 factor:1 | -1 (1.06753) | 1 | 1 |
| G: -5684.20830 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.50952 HOMO: -6.50896 LUMO: 1.88303 factor:1 | -1 (1.06448) | -1 | -1 |
| G: -5684.20830 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.57098 HOMO: -6.60420 LUMO: 2.05990 factor:1 | -1 (0.00302) | 1 | 1 |
| G: -5684.20830 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.53598 HOMO: -7.14299 LUMO: 2.07351 factor:1 | -1 (0.03801) | 1 | 1 |
| G: -5684.20830 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.56380 HOMO: -7.06408 LUMO: 1.81228 factor:1 | -1 (1.01020) | 1 | 1 |
| G: -5684.20830 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.54232 HOMO: -6.67495 LUMO: 1.79595 factor:1 | -1 (0.03167) | 1 | 1 |
| G: -5684.20830 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.68331 HOMO: -6.45182 LUMO: 2.15786 factor:1 | 1 (-0.10931) | -1 | -1 |
| G: -5684.20830 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.55103 HOMO: -6.93346 LUMO: 2.45719 factor:1 | -1 (0.02297) | 1 | 1 |
| G: -5684.20830 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.59671 HOMO: -6.50080 LUMO: 2.08167 factor:1 | 1 (-1.02271) | -1 | -1 |
| G: -5684.20830 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.47935 HOMO: -6.83550 LUMO: -0.67484 factor:1 | 1 (-0.90535) | -1 | -1 |
| G: -5684.20830 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.28335 HOMO: -7.04231 LUMO: 0.54151 factor:1 | 1 (-0.70935) | -1 | -1 |
| G: -5684.20830 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.18451 HOMO: -6.79740 LUMO: 1.91296 factor:1 | 1 (-0.61051) | -1 | -1 |
| G: -5684.20830 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.70958 HOMO: -7.35796 LUMO: -1.04220 factor:1 | 1 (-1.13559) | -1 | -1 |
| G: -5684.20830 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.50871 HOMO: -6.62597 LUMO: -0.44082 factor:1 | 1 (-0.93471) | -1 | -1 |
| G: -5684.20830 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.34256 HOMO: -6.45182 LUMO: -0.20409 factor:1 | 1 (-0.76856) | -1 | -1 |
| G: -5684.20830 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.24022 HOMO: -6.51168 LUMO: -0.23130 factor:1 | 1 (-0.66622) | -1 | -1 |
| G: -5684.20830 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.15262 HOMO: -7.14027 LUMO: 0.49797 factor:1 | 1 (-0.57862) | -1 | -1 |
| G: -5684.20830 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.47593 HOMO: -7.55660 LUMO: 0.24762 factor:1 | -1 (0.09807) | -1 | -1 |
| G: -5684.20830 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.45310 HOMO: -6.88992 LUMO: -0.64763 factor:1 | -1 (0.12090) | -1 | -1 |
| G: -5684.20830 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.41838 HOMO: -6.72665 LUMO: -0.45987 factor:1 | -1 (0.15562) | -1 | -1 |
| G: -5684.20830 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.49350 HOMO: -6.72121 LUMO: -0.58232 factor:1 | 1 (-0.91950) | -1 | -1 |
| G: -5684.20830 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.80432 HOMO: -7.26816 LUMO: 0.32926 factor:1 | -1 (0.76967) | -1 | -1 |
| G: -5684.20830 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.80944 HOMO: -6.57155 LUMO: -0.53606 factor:1 | -1 (0.76456) | -1 | -1 |
| G: -5684.20830 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.27748 HOMO: -6.50896 LUMO: -0.43810 factor:1 | -1 (0.29652) | -1 | -1 |
| G: -5684.20830 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.15233 HOMO: -6.73210 LUMO: -0.51430 factor:1 | -1 (0.42167) | -1 | -1 |
| G: -5684.20830 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.15496 HOMO: -6.77019 LUMO: -0.62858 factor:1 | 1 (-0.58096) | -1 | -1 |
| G: -5684.20830 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.10563 HOMO: -6.82462 LUMO: -0.67484 factor:1 | 1 (-0.53163) | -1 | -1 |
| G: -5684.20830 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.16109 HOMO: -6.79740 LUMO: -0.55511 factor:1 | -1 (0.41291) | -1 | -1 |
| G: -5684.20830 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.42871 HOMO: -6.79740 LUMO: -0.67756 factor:1 | 1 (-0.85471) | -1 | -1 |
| G: -5684.20830 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.54893 HOMO: -6.75114 LUMO: -0.55239 factor:1 | 1 (-0.97493) | -1 | -1 |
| G: -5684.20830 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.45943 HOMO: -6.49536 LUMO: -0.25307 factor:1 | 1 (-0.88543) | -1 | -1 |
| G: -5684.20830 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.31450 HOMO: -6.48992 LUMO: -0.25034 factor:1 | 1 (-0.74050) | -1 | -1 |
| G: -5684.20830 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.51701 HOMO: -6.52801 LUMO: -0.28028 factor:1 | 1 (-0.94301) | -1 | -1 |
| G: -5684.20830 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.89745 HOMO: -7.22462 LUMO: 0.52518 factor:1 | 1 (-1.32345) | -1 | -1 |
| G: -5684.20830 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.44397 HOMO: -6.59332 LUMO: -0.27211 factor:1 | 1 (-0.86998) | -1 | -1 |
| G: -5684.20830 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.44050 HOMO: -6.57427 LUMO: -0.16871 factor:1 | -1 (0.13350) | -1 | -1 |
| G: -5684.20830 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.26409 HOMO: -6.71033 LUMO: 1.59187 factor:1 | -1 (0.30991) | -1 | -1 |
| G: -5684.20830 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.01034 HOMO: -6.72121 LUMO: 2.00004 factor:1 | -1 (0.56366) | -1 | -1 |
| G: -5684.20830 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.01470 HOMO: -6.61509 LUMO: 1.55921 factor:1 | -1 (0.55930) | -1 | -1 |
| G: -5684.20830 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.60766 HOMO: -6.55250 LUMO: 1.73064 factor:1 | 1 (-0.03366) | -1 | -1 |
| G: -5684.20830 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.19704 HOMO: -6.66135 LUMO: 2.02181 factor:1 | -1 (0.37696) | -1 | -1 |
| G: -5684.20830 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.87902 HOMO: -6.84911 LUMO: 1.98099 factor:1 | -1 (0.69498) | -1 | -1 |
| G: -5684.20830 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.09848 HOMO: -6.66679 LUMO: 1.98371 factor:1 | -1 (0.47552) | -1 | -1 |
| G: -5684.20830 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.29571 HOMO: -6.67495 LUMO: 2.04085 factor:1 | -1 (0.27829) | -1 | -1 |
| G: -5684.20830 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.62634 HOMO: -6.89809 LUMO: 1.95106 factor:1 | -1 (0.94766) | -1 | -1 |
| G: -5684.20830 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.76268 HOMO: -6.50352 LUMO: 1.88847 factor:1 | 1 (-0.18868) | -1 | -1 |
| G: -5684.20830 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.73544 HOMO: -6.93618 LUMO: 2.00004 factor:1 | 1 (-0.16145) | -1 | -1 |
| G: -5684.20830 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.75125 HOMO: -6.50896 LUMO: 1.73609 factor:1 | 1 (-0.17725) | -1 | -1 |
| G: -5684.20830 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.72184 HOMO: -6.69672 LUMO: 2.37283 factor:1 | 1 (-0.14784) | -1 | -1 |
| G: -5684.20830 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.16650 HOMO: -6.65591 LUMO: 2.20684 factor:1 | 1 (-0.59250) | -1 | -1 |
| G: -5684.20830 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.28207 HOMO: -6.23957 LUMO: 1.78507 factor:1 | 1 (-0.70807) | -1 | -1 |
| G: -5684.20830 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.49375 HOMO: -6.35114 LUMO: 1.92112 factor:1 | -1 (0.08025) | -1 | -1 |
| G: -5684.20830 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.32676 HOMO: -6.53617 LUMO: 1.75241 factor:1 | -1 (0.24724) | -1 | -1 |
| G: -5684.20830 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.05926 HOMO: -6.60420 LUMO: 1.78779 factor:1 | 1 (-0.48526) | -1 | -1 |
| G: -5684.20830 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.92960 HOMO: -7.40422 LUMO: -0.97145 factor:1 | 1 (-0.35560) | -1 | -1 |
| G: -5684.20830 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.84792 HOMO: -6.80013 LUMO: -0.69117 factor:1 | -1 (0.72608) | -1 | -1 |
| G: -5684.20830 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.39598 HOMO: -6.68040 LUMO: -0.47076 factor:1 | -1 (0.17802) | -1 | -1 |
| G: -5684.20830 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.02911 HOMO: -7.20285 LUMO: -0.66124 factor:1 | 1 (-0.45511) | -1 | -1 |
| G: -5684.20830 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.82796 HOMO: -6.82734 LUMO: -0.60137 factor:1 | 1 (-0.25396) | -1 | -1 |
| G: -5684.20830 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.86294 HOMO: -7.18653 LUMO: 0.59321 factor:1 | -1 (0.71106) | -1 | -1 |
| G: -5684.20830 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.17417 HOMO: -7.29265 LUMO: 0.48164 factor:1 | 1 (-0.60017) | -1 | -1 |
| G: -5684.20830 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.74466 HOMO: -6.63414 LUMO: -0.25034 factor:1 | 1 (-1.17066) | -1 | -1 |
| G: -5684.20830 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.87119 HOMO: -7.20285 LUMO: 0.53879 factor:1 | 1 (-1.29719) | -1 | -1 |
| G: -5684.20830 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.62169 HOMO: -6.46815 LUMO: -0.21769 factor:1 | 1 (-1.04769) | -1 | -1 |
| G: -5684.20830 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.58942 HOMO: -6.57971 LUMO: -0.18776 factor:1 | 1 (-1.01542) | -1 | -1 |
| G: -5684.20830 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.96635 HOMO: -6.90897 LUMO: 1.91296 factor:1 | 1 (-1.39235) | -1 | -1 |
| G: -5684.20830 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.47886 HOMO: -6.67495 LUMO: 2.04358 factor:1 | 1 (-0.90486) | -1 | -1 |
| G: -5684.20830 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.00122 HOMO: -6.94162 LUMO: 1.73881 factor:1 | 1 (-0.42722) | -1 | -1 |
| G: -5684.20830 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.24010 HOMO: -6.73482 LUMO: 1.95922 factor:1 | 1 (-1.66610) | -1 | -1 |
| G: -5684.20830 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.16113 HOMO: -6.70489 LUMO: 2.04358 factor:1 | 1 (-1.58713) | -1 | -1 |
| G: -5684.20830 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.26298 HOMO: -7.04231 LUMO: 1.79323 factor:1 | 1 (-1.68898) | -1 | -1 |
| G: -5684.20830 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.65347 HOMO: -6.68584 LUMO: 1.60275 factor:1 | 1 (-1.07948) | -1 | -1 |
| G: -5684.20830 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.93051 HOMO: -6.40556 LUMO: 1.45581 factor:1 | 1 (-1.35651) | -1 | -1 |
| G: -5684.20830 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.85304 HOMO: -6.94979 LUMO: 2.16603 factor:1 | 1 (-1.27904) | -1 | -1 |
| G: -5684.20830 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.91734 HOMO: -6.84911 LUMO: 1.89935 factor:1 | 1 (-1.34334) | -1 | -1 |
| G: -5684.20830 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.40048 HOMO: -6.22052 LUMO: 1.57282 factor:1 | 1 (-1.82648) | -1 | -1 |
| G: -5684.20830 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.95217 HOMO: -6.51168 LUMO: 2.10072 factor:1 | 1 (-1.37818) | -1 | -1 |
| G: -5684.20830 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.83091 HOMO: -7.03686 LUMO: 2.12249 factor:1 | 1 (-2.25691) | -1 | -1 |
| G: -5684.20830 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.86368 HOMO: -6.84094 LUMO: 1.63268 factor:1 | 1 (-1.28968) | -1 | -1 |
| G: -5684.20830 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.62656 HOMO: -6.75387 LUMO: 1.72248 factor:1 | 1 (-1.05256) | -1 | -1 |
| G: -5684.20830 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.38457 HOMO: -6.86271 LUMO: 1.68711 factor:1 | 1 (-0.81057) | -1 | -1 |
| G: -5684.20830 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.24693 HOMO: -6.84094 LUMO: 2.02997 factor:1 | 1 (-1.67293) | -1 | -1 |
| G: -5684.20830 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.17305 HOMO: -6.80557 LUMO: 2.02725 factor:1 | 1 (-1.59905) | -1 | -1 |
| G: -5684.20830 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.06690 HOMO: -6.38651 LUMO: 1.53472 factor:1 | 1 (-1.49290) | -1 | -1 |
| G: -5684.20830 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.75612 HOMO: -7.51306 LUMO: 0.28572 factor:1 | 1 (-1.18212) | -1 | -1 |
| G: -5684.20830 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.90466 HOMO: -6.97972 LUMO: -0.74287 factor:1 | 1 (-1.33066) | -1 | -1 |
| G: -5684.20830 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.23142 HOMO: -6.83822 LUMO: -0.65852 factor:1 | 1 (-1.65742) | -1 | -1 |
| G: -5684.20830 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.47918 HOMO: -6.71305 LUMO: -0.49525 factor:1 | 1 (-1.90518) | -1 | -1 |
| G: -5684.20830 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.58718 HOMO: -6.60692 LUMO: -0.22313 factor:1 | 1 (-2.01318) | -1 | -1 |
| G: -5684.20830 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11951.12009 HOMO: -7.20013 LUMO: 0.55239 factor:1 | 1 (-2.54609) | -1 | -1 |
| G: -5684.20830 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.04544 HOMO: -6.60420 LUMO: -0.28028 factor:1 | 1 (-0.47144) | -1 | -1 |
| G: -5684.20830 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.08476 HOMO: -6.69128 LUMO: -0.30477 factor:1 | 1 (-0.51076) | -1 | -1 |
| G: -5684.20830 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.08168 HOMO: -6.65591 LUMO: -0.25579 factor:1 | 1 (-0.50768) | -1 | -1 |
| G: -5684.20830 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.65192 HOMO: -6.69128 LUMO: 1.70888 factor:1 | 1 (-1.07792) | -1 | -1 |
| G: -5684.20830 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.82358 HOMO: -6.50080 LUMO: 1.87759 factor:1 | 1 (-0.24958) | -1 | -1 |
| G: -5684.20830 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.54094 HOMO: -6.85727 LUMO: 1.99187 factor:1 | -1 (0.03306) | -1 | -1 |
| G: -5684.20830 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.62264 HOMO: -6.58788 LUMO: 1.79051 factor:1 | 1 (-1.04865) | -1 | -1 |
| G: -5684.20830 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.66006 HOMO: -6.64230 LUMO: 2.16058 factor:1 | 1 (-1.08606) | -1 | -1 |
| G: -5684.20830 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.64218 HOMO: -6.58788 LUMO: 2.10616 factor:1 | 1 (-1.06818) | -1 | -1 |
| G: -5684.20830 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.74107 HOMO: -7.01782 LUMO: 2.13609 factor:1 | 1 (-1.16707) | -1 | -1 |
| G: -5684.20830 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.89977 HOMO: -6.31304 LUMO: 2.31841 factor:1 | 1 (-0.32577) | -1 | -1 |
| G: -5684.20830 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.01994 HOMO: -6.94979 LUMO: 2.07895 factor:1 | 1 (-0.44594) | -1 | -1 |
| G: -5684.20830 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.02046 HOMO: -6.88992 LUMO: 2.28031 factor:1 | 1 (-0.44646) | -1 | -1 |
| G: -5684.20830 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.26022 HOMO: -6.66407 LUMO: 2.07623 factor:1 | 1 (-0.68622) | -1 | -1 |
| G: -5684.20830 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.62248 HOMO: -6.52529 LUMO: 1.70071 factor:1 | 1 (-1.04848) | -1 | -1 |
| G: -5684.20830 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.44830 HOMO: -6.58788 LUMO: 1.57282 factor:1 | 1 (-0.87430) | -1 | -1 |
| G: -5684.20830 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.33829 HOMO: -6.55250 LUMO: 1.95378 factor:1 | 1 (-0.76429) | -1 | -1 |
| G: -5684.20830 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.70806 HOMO: -6.24773 LUMO: 1.77962 factor:1 | 1 (-1.13406) | -1 | -1 |
| G: -5684.20830 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.60724 HOMO: -6.31304 LUMO: 2.18507 factor:1 | 1 (-1.03324) | -1 | -1 |
| G: -5684.20830 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.73890 HOMO: -6.18243 LUMO: 2.01636 factor:1 | 1 (-0.16490) | -1 | -1 |
| G: -5684.20830 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.67327 HOMO: -6.99877 LUMO: 2.14970 factor:1 | 1 (-0.09927) | -1 | -1 |
| G: -5684.20830 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.03022 HOMO: -6.72665 LUMO: 2.07079 factor:1 | 1 (-1.45622) | -1 | -1 |
| G: -5684.20830 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.13577 HOMO: -6.36202 LUMO: 2.17419 factor:1 | 1 (-1.56177) | -1 | -1 |
| G: -5684.20830 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.11042 HOMO: -6.78652 LUMO: 2.05718 factor:1 | 1 (-0.53642) | -1 | -1 |
| G: -5684.20830 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.00807 HOMO: -6.87360 LUMO: 2.34290 factor:1 | 1 (-0.43408) | -1 | -1 |
| G: -5684.20830 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.83161 HOMO: -6.62053 LUMO: 1.89391 factor:1 | 1 (-0.25761) | -1 | -1 |
| G: -5684.20830 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.77990 HOMO: -6.58788 LUMO: 1.83133 factor:1 | 1 (-1.20590) | -1 | -1 |
| G: -5684.20830 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.67927 HOMO: -7.08584 LUMO: 1.91568 factor:1 | 1 (-1.10527) | 1 | 1 |
| G: -5684.20830 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.77745 HOMO: -6.56883 LUMO: 1.81228 factor:1 | 1 (-1.20345) | -1 | -1 |
| G: -5684.20830 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.36210 HOMO: -6.66135 LUMO: 1.92384 factor:1 | -1 (0.21190) | -1 | -1 |
| G: -5684.20830 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.20795 HOMO: -6.64502 LUMO: 2.15786 factor:1 | -1 (0.36605) | -1 | -1 |
| G: -5684.20830 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.85490 HOMO: -6.71305 LUMO: 1.91840 factor:1 | 1 (-0.28090) | -1 | -1 |
| G: -5684.20830 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.12888 HOMO: -6.44094 LUMO: 1.74425 factor:1 | -1 (0.44512) | -1 | -1 |
| G: -5684.20830 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.95295 HOMO: -6.51985 LUMO: 1.84221 factor:1 | -1 (0.62105) | -1 | -1 |
| G: -5684.20830 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.02666 HOMO: -6.63414 LUMO: -0.24762 factor:1 | 1 (-0.45266) | -1 | -1 |
| G: -5684.20830 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.88834 HOMO: -6.60420 LUMO: -0.22585 factor:1 | 1 (-0.31435) | -1 | -1 |
| G: -5684.20830 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.78377 HOMO: -7.19741 LUMO: 0.58232 factor:1 | 1 (-0.20977) | -1 | -1 |
| G: -5684.20830 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.26863 HOMO: -6.77019 LUMO: -0.56872 factor:1 | -1 (0.30537) | -1 | -1 |
| G: -5684.20830 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.06980 HOMO: -7.46136 LUMO: 0.28844 factor:1 | -1 (0.50420) | -1 | -1 |
| G: -5684.20830 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.94962 HOMO: -6.60420 LUMO: -0.54151 factor:1 | 1 (-0.37563) | -1 | -1 |
| G: -5684.20830 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.08749 HOMO: -6.53890 LUMO: -0.46531 factor:1 | -1 (0.48651) | -1 | -1 |
| G: -5684.20830 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.81322 HOMO: -6.81645 LUMO: -0.57144 factor:1 | -1 (0.76078) | -1 | -1 |
| G: -5684.20830 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.93681 HOMO: -7.48041 LUMO: 0.28572 factor:1 | 1 (-0.36281) | -1 | -1 |
| G: -5684.20830 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.72965 HOMO: -6.75659 LUMO: -0.45715 factor:1 | 1 (-0.15565) | -1 | -1 |
| G: -5684.20830 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.86720 HOMO: -6.66135 LUMO: -0.41906 factor:1 | 1 (-0.29320) | -1 | -1 |
| G: -5684.20830 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.68894 HOMO: -6.55794 LUMO: -0.27483 factor:1 | 1 (-0.11494) | -1 | -1 |
| G: -5684.20830 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.73958 HOMO: -7.07496 LUMO: -0.63403 factor:1 | 1 (-0.16558) | -1 | -1 |
| G: -5684.20830 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.91262 HOMO: -7.12394 LUMO: 0.53334 factor:1 | 1 (-0.33862) | -1 | -1 |
| G: -5684.20830 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.71215 HOMO: -6.53617 LUMO: -0.25579 factor:1 | 1 (-0.13815) | -1 | -1 |
| G: -5684.20830 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.95436 HOMO: -6.50896 LUMO: -0.25034 factor:1 | 1 (-0.38036) | -1 | -1 |
| G: -5684.20830 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.39799 HOMO: -7.17564 LUMO: -0.68573 factor:1 | 1 (-0.82399) | -1 | -1 |
| G: -5684.20830 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.68746 HOMO: -6.53617 LUMO: -0.30749 factor:1 | 1 (-1.11346) | -1 | -1 |
| G: -5684.20830 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.36536 HOMO: -6.55522 LUMO: -0.30749 factor:1 | 1 (-0.79136) | -1 | -1 |
| G: -5684.20830 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.52879 HOMO: -7.05591 LUMO: -0.71022 factor:1 | 1 (-0.95479) | -1 | -1 |
| G: -5684.20830 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.98227 HOMO: -7.17564 LUMO: -0.69933 factor:1 | 1 (-1.40827) | -1 | -1 |
| G: -5684.20830 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.11447 HOMO: -6.78380 LUMO: -0.67756 factor:1 | 1 (-0.54047) | -1 | -1 |
| G: -5684.20830 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.89874 HOMO: -6.62325 LUMO: 2.02725 factor:1 | 1 (-0.32474) | -1 | -1 |
| G: -5684.20830 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.07295 HOMO: -6.63414 LUMO: 1.91296 factor:1 | 1 (-0.49895) | -1 | -1 |
| G: -5684.20830 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.44016 HOMO: -6.83278 LUMO: 1.65717 factor:1 | 1 (-0.86617) | -1 | -1 |
| G: -5684.20830 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.84526 HOMO: -6.66407 LUMO: 1.95650 factor:1 | 1 (-1.27126) | -1 | -1 |
| G: -5684.20830 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.62126 HOMO: -6.61237 LUMO: 2.11432 factor:1 | 1 (-1.04726) | -1 | -1 |
| G: -5684.20830 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.73873 HOMO: -6.62053 LUMO: 2.09256 factor:1 | 1 (-1.16473) | -1 | -1 |
| G: -5684.20830 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.82184 HOMO: -6.78652 LUMO: 2.13609 factor:1 | 1 (-0.24784) | -1 | -1 |
| G: -5684.20830 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.23223 HOMO: -6.94707 LUMO: 1.81772 factor:1 | 1 (-1.65823) | -1 | -1 |
| G: -5684.20830 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.31047 HOMO: -6.85183 LUMO: 2.12793 factor:1 | 1 (-1.73647) | -1 | -1 |
| G: -5684.20830 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.78856 HOMO: -6.81101 LUMO: 1.83949 factor:1 | 1 (-0.21456) | -1 | -1 |
| G: -5684.20830 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.52080 HOMO: -6.98788 LUMO: 2.16058 factor:1 | -1 (0.05320) | -1 | -1 |
| G: -5684.20830 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.79683 HOMO: -6.62869 LUMO: 2.00820 factor:1 | 1 (-0.22283) | -1 | -1 |
| G: -5684.20830 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.63813 HOMO: -6.34025 LUMO: 2.25855 factor:1 | 1 (-1.06413) | -1 | -1 |
| G: -5684.20830 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.88481 HOMO: -6.01372 LUMO: 2.01636 factor:1 | 1 (-0.31081) | -1 | -1 |
| G: -5684.20830 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.85694 HOMO: -6.89264 LUMO: 2.27487 factor:1 | 1 (-0.28294) | -1 | -1 |
| G: -5684.20830 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.13428 HOMO: -6.53073 LUMO: 2.20684 factor:1 | 1 (-0.56028) | -1 | -1 |
| G: -5684.20830 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.26672 HOMO: -6.83278 LUMO: 1.53744 factor:1 | 1 (-0.69272) | -1 | -1 |
| G: -5684.20830 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.14950 HOMO: -6.41917 LUMO: 1.82316 factor:1 | -1 (0.42450) | -1 | -1 |
| G: -5684.20830 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.74450 HOMO: -6.56339 LUMO: 1.63813 factor:1 | 1 (-1.17050) | -1 | -1 |
| G: -5684.20830 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.82736 HOMO: -6.88992 LUMO: 1.65173 factor:1 | 1 (-1.25336) | -1 | -1 |
| G: -5684.20830 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.65084 HOMO: -6.63141 LUMO: 1.92112 factor:1 | 1 (-0.07684) | -1 | -1 |
| G: -5684.20830 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.50148 HOMO: -6.83822 LUMO: 1.88847 factor:1 | -1 (0.07252) | -1 | -1 |
| G: -5684.20830 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.66557 HOMO: -6.84638 LUMO: 1.90480 factor:1 | 1 (-0.09157) | -1 | -1 |
| G: -5684.20830 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.19164 HOMO: -6.82462 LUMO: 1.70888 factor:1 | 1 (-0.61764) | -1 | -1 |
| G: -5684.20830 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.49478 HOMO: -6.82734 LUMO: 2.12521 factor:1 | 1 (-0.92078) | -1 | -1 |
| G: -5684.20830 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.01218 HOMO: -6.94435 LUMO: 1.87214 factor:1 | 1 (-0.43818) | -1 | -1 |
| G: -5684.20830 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.18710 HOMO: -6.98516 LUMO: 2.51433 factor:1 | 1 (-0.61310) | -1 | -1 |
| G: -5684.20830 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.45800 HOMO: -6.74026 LUMO: 2.15514 factor:1 | -1 (0.11600) | -1 | -1 |
| G: -5684.20830 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.34133 HOMO: -6.93618 LUMO: 2.54426 factor:1 | 1 (-0.76733) | -1 | -1 |
| G: -5684.20830 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.70093 HOMO: -6.28583 LUMO: 2.53610 factor:1 | 1 (-1.12693) | -1 | -1 |
| G: -5684.20830 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.57554 HOMO: -6.56883 LUMO: 1.94834 factor:1 | 1 (-1.00154) | -1 | -1 |
| G: -5684.20830 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.59775 HOMO: -7.08584 LUMO: 1.99187 factor:1 | 1 (-1.02375) | 1 | 1 |
| G: -5684.20830 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.47276 HOMO: -6.19059 LUMO: 1.99732 factor:1 | 1 (-0.89876) | -1 | -1 |
| G: -5684.20830 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.36985 HOMO: -6.78108 LUMO: 2.03813 factor:1 | 1 (-0.79585) | -1 | -1 |
| G: -5684.20830 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.38307 HOMO: -6.82189 LUMO: 1.77418 factor:1 | 1 (-1.80907) | -1 | -1 |
| G: -5684.20830 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.38922 HOMO: -6.45454 LUMO: 1.78779 factor:1 | 1 (-1.81522) | -1 | -1 |
| G: -5684.20830 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.24206 HOMO: -6.84366 LUMO: 1.77690 factor:1 | 1 (-1.66806) | -1 | -1 |
| G: -5684.20830 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.09691 HOMO: -6.74026 LUMO: 1.67622 factor:1 | 1 (-1.52291) | -1 | -1 |
| G: -5684.20830 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.06039 HOMO: -6.76475 LUMO: 2.40277 factor:1 | 1 (-1.48639) | -1 | -1 |
| G: -5684.20830 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.87509 HOMO: -6.65863 LUMO: 1.86670 factor:1 | 1 (-0.30109) | -1 | -1 |
| G: -5684.20830 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.89858 HOMO: -6.50080 LUMO: 1.93201 factor:1 | 1 (-0.32458) | -1 | -1 |
| G: -5684.20830 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.04008 HOMO: -6.34842 LUMO: 1.70888 factor:1 | 1 (-0.46608) | -1 | -1 |
| G: -5684.20830 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.87327 HOMO: -6.60692 LUMO: 2.20140 factor:1 | 1 (-0.29927) | -1 | -1 |
| G: -5684.20830 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.16849 HOMO: -6.74026 LUMO: 2.14970 factor:1 | 1 (-0.59449) | -1 | -1 |
| G: -5684.20830 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.65922 HOMO: -6.63686 LUMO: 2.17419 factor:1 | 1 (-1.08522) | -1 | -1 |
| G: -5684.20830 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.66847 HOMO: -6.81917 LUMO: 2.10072 factor:1 | 1 (-1.09447) | -1 | -1 |
| G: -5684.20830 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.73250 HOMO: -6.92802 LUMO: 2.04358 factor:1 | 1 (-1.15850) | -1 | -1 |
| G: -5684.20830 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.32577 HOMO: -6.56067 LUMO: -0.47620 factor:1 | 1 (-0.75177) | -1 | -1 |
| G: -5684.20830 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.48270 HOMO: -6.56611 LUMO: -0.77008 factor:1 | 1 (-0.90870) | -1 | -1 |
| G: -5684.20830 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.85749 HOMO: -6.78380 LUMO: -0.64763 factor:1 | 1 (-0.28349) | -1 | -1 |
| G: -5684.20830 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.65437 HOMO: -6.51985 LUMO: -0.24490 factor:1 | 1 (-1.08037) | -1 | -1 |
| G: -5684.20830 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.11479 HOMO: -6.52529 LUMO: -0.27483 factor:1 | 1 (-1.54079) | -1 | -1 |
| G: -5684.20830 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.10159 HOMO: -7.10489 LUMO: -0.62586 factor:1 | 1 (-1.52759) | -1 | -1 |
| G: -5684.20830 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.60343 HOMO: -7.18108 LUMO: 0.48980 factor:1 | 1 (-1.02943) | -1 | -1 |
| G: -5684.20830 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.64923 HOMO: -7.14299 LUMO: -0.63947 factor:1 | 1 (-1.07523) | -1 | -1 |
| G: -5684.20830 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.80091 HOMO: -6.70761 LUMO: -0.54423 factor:1 | 1 (-1.22691) | -1 | -1 |
| G: -5684.20830 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.45312 HOMO: -7.32258 LUMO: -1.03675 factor:1 | 1 (-0.87912) | -1 | -1 |
| G: -5684.20830 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.45739 HOMO: -6.65046 LUMO: -0.41361 factor:1 | 1 (-0.88339) | -1 | -1 |
| G: -5684.20830 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.35052 HOMO: -6.76475 LUMO: -0.60137 factor:1 | 1 (-1.77652) | -1 | -1 |
| G: -5684.20830 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.38366 HOMO: -6.77836 LUMO: -0.54423 factor:1 | 1 (-1.80967) | -1 | -1 |
| G: -5684.20830 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.53662 HOMO: -7.52395 LUMO: 0.26395 factor:1 | 1 (-1.96262) | -1 | -1 |
| G: -5684.20830 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.78076 HOMO: -6.93890 LUMO: -0.72382 factor:1 | 1 (-2.20676) | -1 | -1 |
| G: -5684.20830 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.20578 HOMO: -6.72938 LUMO: -0.47348 factor:1 | 1 (-1.63179) | -1 | -1 |
| G: -5684.20830 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.87400 HOMO: -6.66951 LUMO: -0.40817 factor:1 | 1 (-1.30000) | -1 | -1 |
| G: -5684.20830 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.81576 HOMO: -6.60420 LUMO: -0.19320 factor:1 | 1 (-1.24176) | -1 | -1 |
| G: -5684.20830 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.86589 HOMO: -6.67495 LUMO: -0.27211 factor:1 | 1 (-1.29189) | -1 | -1 |
| G: -5684.20830 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.65640 HOMO: -7.23823 LUMO: -0.62858 factor:1 | 1 (-2.08241) | -1 | -1 |
| G: -5684.20830 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.77265 HOMO: -7.27088 LUMO: 0.53334 factor:1 | 1 (-2.19865) | -1 | -1 |
| G: -5684.20830 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.06767 HOMO: -7.20013 LUMO: 0.59049 factor:1 | 1 (-0.49367) | -1 | -1 |
| G: -5684.20830 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.91724 HOMO: -6.60148 LUMO: -0.20953 factor:1 | 1 (-0.34324) | -1 | -1 |
| G: -5684.20830 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.19034 HOMO: -6.69400 LUMO: -0.51974 factor:1 | 1 (-0.61634) | -1 | -1 |
| G: -5684.20830 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.78510 HOMO: -7.40422 LUMO: -0.98777 factor:1 | 1 (-0.21111) | -1 | -1 |
| G: -5684.20830 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.81819 HOMO: -6.88176 LUMO: -0.71022 factor:1 | 1 (-0.24419) | -1 | -1 |
| G: -5684.20830 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.78964 HOMO: -6.86271 LUMO: -0.59321 factor:1 | 1 (-1.21564) | -1 | -1 |
| G: -5684.20830 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.64166 HOMO: -6.73754 LUMO: -0.55239 factor:1 | 1 (-1.06767) | -1 | -1 |
| G: -5684.20830 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.65571 HOMO: -6.71033 LUMO: 1.57010 factor:1 | 1 (-1.08171) | -1 | -1 |
| G: -5684.20830 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.91251 HOMO: -6.69672 LUMO: 1.68711 factor:1 | 1 (-0.33851) | -1 | -1 |
| G: -5684.20830 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.92440 HOMO: -6.67495 LUMO: 2.03813 factor:1 | 1 (-0.35040) | -1 | -1 |
| G: -5684.20830 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.76486 HOMO: -6.54434 LUMO: 1.83677 factor:1 | 1 (-0.19086) | -1 | -1 |
| G: -5684.20830 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.69789 HOMO: -6.57155 LUMO: 1.77146 factor:1 | 1 (-0.12389) | -1 | -1 |
| G: -5684.20830 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.59267 HOMO: -6.76747 LUMO: 1.87759 factor:1 | 1 (-0.01867) | -1 | -1 |
| G: -5684.20830 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.39987 HOMO: -6.58243 LUMO: 1.61364 factor:1 | -1 (0.17413) | -1 | -1 |
| G: -5684.20830 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.66556 HOMO: -6.61781 LUMO: 2.13881 factor:1 | 1 (-1.09156) | -1 | -1 |
| G: -5684.20830 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.42280 HOMO: -6.62597 LUMO: 2.00276 factor:1 | 1 (-0.84880) | -1 | -1 |
| G: -5684.20830 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.27320 HOMO: -7.01237 LUMO: 1.95922 factor:1 | 1 (-0.69920) | -1 | -1 |
| G: -5684.20830 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.92464 HOMO: -7.03959 LUMO: 2.16875 factor:1 | 1 (-1.35064) | -1 | -1 |
| G: -5684.20830 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.94660 HOMO: -6.83278 LUMO: 1.91296 factor:1 | 1 (-0.37261) | -1 | -1 |
| G: -5684.20830 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.95928 HOMO: -6.40012 LUMO: 1.95650 factor:1 | 1 (-0.38529) | -1 | -1 |
| G: -5684.20830 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.58080 HOMO: -6.50080 LUMO: 1.73337 factor:1 | 1 (-0.00680) | -1 | -1 |
| G: -5684.20830 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.05923 HOMO: -6.95795 LUMO: 2.28848 factor:1 | 1 (-0.48523) | -1 | -1 |
| G: -5684.20830 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.46963 HOMO: -6.63686 LUMO: 2.20140 factor:1 | 1 (-0.89564) | -1 | -1 |
| G: -5684.20830 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.79394 HOMO: -6.57427 LUMO: 1.87214 factor:1 | 1 (-1.21994) | -1 | -1 |
| G: -5684.20830 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.36493 HOMO: -6.38379 LUMO: 2.32113 factor:1 | 1 (-0.79093) | -1 | -1 |
| G: -5684.20830 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.81697 HOMO: -6.63958 LUMO: 2.04902 factor:1 | 1 (-0.24297) | -1 | -1 |
| G: -5684.20830 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.47233 HOMO: -6.70216 LUMO: 1.93201 factor:1 | 1 (-0.89833) | -1 | -1 |
| G: -5684.20830 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.68698 HOMO: -6.80557 LUMO: 2.23678 factor:1 | 1 (-0.11298) | -1 | -1 |
| G: -5684.20830 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.02630 HOMO: -6.72938 LUMO: 2.28304 factor:1 | 1 (-1.45230) | -1 | -1 |
| G: -5684.20830 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.08382 HOMO: -6.56067 LUMO: 1.66806 factor:1 | 1 (-1.50982) | -1 | -1 |
| G: -5684.20830 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.79844 HOMO: -6.95523 LUMO: 2.33474 factor:1 | 1 (-0.22444) | -1 | -1 |
| G: -5684.20830 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.75226 HOMO: -6.59876 LUMO: 2.30480 factor:1 | 1 (-0.17826) | -1 | -1 |
| G: -5684.20830 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.78837 HOMO: -6.87360 LUMO: 1.75786 factor:1 | 1 (-0.21437) | -1 | -1 |
| G: -5684.20830 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.48735 HOMO: -7.06408 LUMO: 1.99187 factor:1 | 1 (-0.91335) | 1 | 1 |
| G: -5684.20830 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.15711 HOMO: -6.95795 LUMO: 1.88847 factor:1 | 1 (-0.58311) | -1 | -1 |
| G: -5684.20830 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.81321 HOMO: -6.85455 LUMO: 1.63813 factor:1 | 1 (-0.23922) | -1 | -1 |
| G: -5684.20830 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.70502 HOMO: -7.09129 LUMO: 2.31569 factor:1 | 1 (-0.13102) | 1 | 1 |
| G: -5684.20830 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.68616 HOMO: -6.91441 LUMO: 1.68983 factor:1 | 1 (-0.11217) | -1 | -1 |
| G: -5684.20830 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.43740 HOMO: -6.89809 LUMO: 2.23678 factor:1 | -1 (0.13660) | -1 | -1 |
| G: -5684.20830 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.28014 HOMO: -6.78652 LUMO: 1.98371 factor:1 | -1 (0.29386) | -1 | -1 |
| G: -5684.20830 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.68026 HOMO: -6.94707 LUMO: 2.23678 factor:1 | 1 (-0.10626) | -1 | -1 |
| G: -5684.20830 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.97738 HOMO: -7.07224 LUMO: 2.13337 factor:1 | 1 (-0.40338) | 1 | 1 |
| G: -5684.20830 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.16359 HOMO: -6.94979 LUMO: 2.28031 factor:1 | 1 (-0.58959) | -1 | -1 |
| G: -5684.20830 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.49502 HOMO: -6.60965 LUMO: 2.20412 factor:1 | 1 (-0.92102) | -1 | -1 |
| G: -5684.20830 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.42112 HOMO: -6.87360 LUMO: 2.40277 factor:1 | 1 (-0.84712) | -1 | -1 |
| G: -5684.20830 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.87830 HOMO: -6.92802 LUMO: 1.89663 factor:1 | 1 (-0.30430) | -1 | -1 |
| G: -5684.20830 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.93626 HOMO: -6.88448 LUMO: 2.02725 factor:1 | 1 (-0.36227) | -1 | -1 |
| G: -5684.20830 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.67454 HOMO: -6.69128 LUMO: 1.55105 factor:1 | 1 (-0.10055) | -1 | -1 |
| G: -5684.20830 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.23115 HOMO: -6.54978 LUMO: 1.93201 factor:1 | 1 (-0.65715) | -1 | -1 |
| G: -5684.20830 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.19206 HOMO: -6.19331 LUMO: 1.46941 factor:1 | -1 (0.38194) | -1 | -1 |
| G: -5684.20830 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.52238 HOMO: -6.55794 LUMO: 1.89663 factor:1 | -1 (0.05162) | -1 | -1 |
| G: -5684.20830 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.54438 HOMO: -6.07630 LUMO: 1.94289 factor:1 | 1 (-0.97039) | -1 | -1 |
| G: -5684.20830 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.50648 HOMO: -7.46408 LUMO: 0.31565 factor:1 | 1 (-0.93248) | -1 | -1 |
| G: -5684.20830 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.71387 HOMO: -6.63958 LUMO: -0.61770 factor:1 | 1 (-0.13987) | -1 | -1 |
| G: -5684.20830 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.90279 HOMO: -6.81101 LUMO: -0.57960 factor:1 | 1 (-0.32880) | -1 | -1 |
| G: -5684.20830 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.00614 HOMO: -6.74298 LUMO: -0.57960 factor:1 | 1 (-0.43214) | -1 | -1 |
| G: -5684.20830 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.67196 HOMO: -6.63686 LUMO: -0.42994 factor:1 | 1 (-0.09796) | -1 | -1 |
| G: -5684.20830 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.74900 HOMO: -6.60965 LUMO: -0.41089 factor:1 | 1 (-0.17500) | -1 | -1 |
| G: -5684.20830 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.57808 HOMO: -6.60692 LUMO: -0.80274 factor:1 | 1 (-0.00408) | -1 | -1 |
| G: -5684.20830 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.74723 HOMO: -6.58788 LUMO: -0.78097 factor:1 | 1 (-0.17323) | -1 | -1 |
| G: -5684.20830 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.38939 HOMO: -6.67767 LUMO: -0.48436 factor:1 | 1 (-0.81539) | -1 | -1 |
| G: -5684.20830 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.51508 HOMO: -6.63141 LUMO: -0.40545 factor:1 | 1 (-0.94108) | -1 | -1 |
| G: -5684.20830 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.70011 HOMO: -6.62053 LUMO: -0.83811 factor:1 | 1 (-1.12612) | -1 | -1 |
| G: -5684.20830 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.96257 HOMO: -6.59604 LUMO: -0.35375 factor:1 | 1 (-1.38857) | -1 | -1 |
| G: -5684.20830 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.35793 HOMO: -6.34297 LUMO: -0.39729 factor:1 | 1 (-0.78393) | -1 | -1 |
| G: -5684.20830 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.33355 HOMO: -6.67223 LUMO: 1.97827 factor:1 | 1 (-0.75955) | -1 | -1 |
| G: -5684.20830 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.37065 HOMO: -6.40012 LUMO: 1.89935 factor:1 | -1 (0.20335) | -1 | -1 |
| G: -5684.20830 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.88984 HOMO: -6.74842 LUMO: 1.97283 factor:1 | 1 (-0.31584) | -1 | -1 |
| G: -5684.20830 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.28462 HOMO: -6.76747 LUMO: 2.17147 factor:1 | 1 (-0.71063) | -1 | -1 |
| G: -5684.20830 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.43646 HOMO: -6.72121 LUMO: 1.55649 factor:1 | 1 (-0.86246) | -1 | -1 |
| G: -5684.20830 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.30076 HOMO: -6.97700 LUMO: 2.04085 factor:1 | 1 (-0.72676) | -1 | -1 |
| G: -5684.20830 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.30286 HOMO: -7.06680 LUMO: 2.04085 factor:1 | 1 (-0.72886) | 1 | 1 |
| G: -5684.20830 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.99345 HOMO: -7.09673 LUMO: 2.35106 factor:1 | 1 (-1.41945) | 1 | 1 |
| G: -5684.20830 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.96651 HOMO: -6.83006 LUMO: 2.14970 factor:1 | 1 (-1.39252) | -1 | -1 |
| G: -5684.20830 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.83919 HOMO: -6.72665 LUMO: 2.20140 factor:1 | 1 (-1.26519) | -1 | -1 |
| G: -5684.20830 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.45199 HOMO: -6.77291 LUMO: 2.34562 factor:1 | 1 (-1.87799) | -1 | -1 |
| G: -5684.20830 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11951.25522 HOMO: -6.73754 LUMO: 2.00276 factor:1 | 1 (-2.68122) | -1 | -1 |
| G: -5684.20830 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.74928 HOMO: -7.04231 LUMO: 1.92112 factor:1 | 1 (-2.17528) | -1 | -1 |
| G: -5684.20830 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.93454 HOMO: -6.83822 LUMO: 1.72248 factor:1 | 1 (-1.36054) | -1 | -1 |
| G: -5684.20830 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.86203 HOMO: -6.57971 LUMO: 2.16603 factor:1 | 1 (-0.28803) | -1 | -1 |
| G: -5684.20830 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.79923 HOMO: -6.80013 LUMO: 1.88575 factor:1 | 1 (-0.22523) | -1 | -1 |
| G: -5684.20830 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.93918 HOMO: -6.93618 LUMO: 2.18235 factor:1 | 1 (-0.36518) | -1 | -1 |
| G: -5684.20830 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.81335 HOMO: -6.54706 LUMO: 1.91024 factor:1 | 1 (-0.23935) | -1 | -1 |
| G: -5684.20830 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.93994 HOMO: -7.06952 LUMO: 2.18507 factor:1 | 1 (-0.36594) | 1 | 1 |
| G: -5684.20830 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.78932 HOMO: -7.05047 LUMO: 1.82044 factor:1 | 1 (-0.21532) | -1 | -1 |
| G: -5684.20830 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.88263 HOMO: -6.87632 LUMO: 1.92657 factor:1 | 1 (-0.30863) | -1 | -1 |
| G: -5684.20830 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.72251 HOMO: -6.58788 LUMO: 1.91568 factor:1 | 1 (-1.14851) | -1 | -1 |
| G: -5684.20830 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.65984 HOMO: -7.17292 LUMO: 1.90752 factor:1 | 1 (-1.08584) | 1 | 1 |
| G: -5684.20830 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.60798 HOMO: -6.93890 LUMO: 1.80684 factor:1 | 1 (-1.03398) | -1 | -1 |
| G: -5684.20830 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.48596 HOMO: -7.10761 LUMO: 2.20956 factor:1 | 1 (-0.91196) | 1 | 1 |
| G: -5684.20830 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.76927 HOMO: -6.85727 LUMO: 2.13609 factor:1 | 1 (-0.19527) | -1 | -1 |
| G: -5684.20830 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.48997 HOMO: -6.64502 LUMO: 1.38506 factor:1 | -1 (0.08403) | -1 | -1 |
| G: -5684.20830 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.83234 HOMO: -6.87360 LUMO: 1.15648 factor:1 | 1 (-0.25834) | -1 | -1 |
| G: -5684.20830 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.07945 HOMO: -6.67223 LUMO: 2.07351 factor:1 | 1 (-0.50545) | -1 | -1 |
| G: -5684.20830 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.73291 HOMO: -6.29671 LUMO: 2.43270 factor:1 | 1 (-0.15891) | -1 | -1 |
| G: -5684.20830 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.46964 HOMO: -6.90897 LUMO: 2.28848 factor:1 | -1 (0.10436) | -1 | -1 |
| G: -5684.20830 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.95945 HOMO: -7.04231 LUMO: 1.70071 factor:1 | 1 (-0.38545) | -1 | -1 |
| G: -5684.20830 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.39544 HOMO: -6.69944 LUMO: 1.94834 factor:1 | -1 (0.17856) | -1 | -1 |
| G: -5684.20830 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.22284 HOMO: -6.56067 LUMO: 2.20956 factor:1 | -1 (0.35116) | -1 | -1 |
| G: -5684.20830 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.48953 HOMO: -6.65046 LUMO: 2.06807 factor:1 | 1 (-0.91553) | -1 | -1 |
| G: -5684.20830 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.35075 HOMO: -7.08584 LUMO: 1.98915 factor:1 | 1 (-0.77675) | 1 | 1 |
| G: -5684.20830 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.37796 HOMO: -6.69400 LUMO: 2.09256 factor:1 | 1 (-0.80396) | -1 | -1 |
| G: -5684.20830 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.22745 HOMO: -6.62869 LUMO: 2.16331 factor:1 | 1 (-0.65345) | -1 | -1 |
| G: -5684.20830 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.94984 HOMO: -6.85183 LUMO: 2.16058 factor:1 | 1 (-0.37584) | -1 | -1 |
| G: -5684.20830 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.91335 HOMO: -6.54706 LUMO: 1.92384 factor:1 | 1 (-0.33935) | -1 | -1 |
| G: -5684.20830 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.99838 HOMO: -6.84366 LUMO: 2.48984 factor:1 | 1 (-1.42438) | -1 | -1 |
| G: -5684.20830 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.34822 HOMO: -6.77291 LUMO: 2.46263 factor:1 | 1 (-0.77422) | -1 | -1 |
| G: -5684.20830 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.60183 HOMO: -7.01782 LUMO: 2.31025 factor:1 | 1 (-1.02783) | -1 | -1 |
| G: -5684.20830 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.68177 HOMO: -6.94707 LUMO: 2.29664 factor:1 | 1 (-1.10778) | -1 | -1 |
| G: -5684.20830 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.12342 HOMO: -6.64230 LUMO: 1.97283 factor:1 | 1 (-1.54942) | -1 | -1 |
| G: -5684.20830 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.57549 HOMO: -6.47359 LUMO: 2.20412 factor:1 | 1 (-1.00149) | -1 | -1 |
| G: -5684.20830 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.49695 HOMO: -6.90625 LUMO: 1.92384 factor:1 | 1 (-1.92295) | -1 | -1 |
| G: -5684.20830 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.48253 HOMO: -7.17020 LUMO: 2.06807 factor:1 | 1 (-0.90853) | 1 | 1 |
| G: -5684.20830 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.64248 HOMO: -6.65046 LUMO: 2.20956 factor:1 | 1 (-1.06848) | -1 | -1 |
| G: -5684.20830 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.67471 HOMO: -7.07496 LUMO: 1.82861 factor:1 | 1 (-0.10071) | 1 | 1 |
| G: -5684.20830 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.06865 HOMO: -6.83006 LUMO: 2.14970 factor:1 | 1 (-0.49465) | -1 | -1 |
| G: -5684.20830 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.84614 HOMO: -6.92802 LUMO: 1.99187 factor:1 | 1 (-0.27214) | -1 | -1 |
| G: -5684.20830 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.56019 HOMO: -6.69672 LUMO: 2.36739 factor:1 | 1 (-0.98620) | -1 | -1 |
| G: -5684.20830 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.54392 HOMO: -7.13755 LUMO: 2.00276 factor:1 | 1 (-0.96992) | 1 | 1 |
| G: -5684.20830 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.34040 HOMO: -6.92530 LUMO: 2.25582 factor:1 | 1 (-1.76640) | -1 | -1 |
| G: -5684.20830 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.60249 HOMO: -6.77564 LUMO: 1.97827 factor:1 | 1 (-0.02849) | -1 | -1 |
| G: -5684.20830 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.84632 HOMO: -6.87904 LUMO: 1.60003 factor:1 | 1 (-1.27232) | -1 | -1 |
| G: -5684.20830 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.62415 HOMO: -6.62869 LUMO: 1.90480 factor:1 | 1 (-0.05015) | -1 | -1 |
| G: -5684.20830 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.73290 HOMO: -6.71033 LUMO: 1.54833 factor:1 | 1 (-1.15891) | -1 | -1 |
| G: -5684.20830 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.56854 HOMO: -6.74298 LUMO: 1.47486 factor:1 | -1 (1.00546) | -1 | -1 |
| G: -5684.20830 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.39724 HOMO: -6.77019 LUMO: 1.90480 factor:1 | -1 (1.17676) | -1 | -1 |
| G: -5684.20830 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.44453 HOMO: -6.70489 LUMO: 1.99459 factor:1 | -1 (0.12947) | -1 | -1 |