乙二醇作为反应物的反应表19-11

说明：  
 Gibbs自由能判据: ‘1’代表从热力学角度利于反应正向进行；‘-1’代表从热力学角度不利于反应正向进行。  
 前线轨道理论判据: ‘1’代表基于前线轨道理论利于反应正向进行；‘-1’代表基于前线轨道理论不利于反应正向进行。  
 是否同时满足: ‘1’代表同时满足Gibbs和前线轨道理论判据，利于反应正向进行；‘-1’代表不同时满足上述两判据。  
 数据来源：所有原始属性数据计算方法均为 B3LYP/6-31G(2df,p)，单位均为eV。

|  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- |
| 反应物A | 反应物B | 产物C | Gibbs自由能判据(ΔG) | 前线轨道理论判据 | 是否同时满足 |
| G: -6289.12860 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.38168 HOMO: -6.91169 LUMO: -0.53879 factor:1 | 1 (-1.88738) | -1 | -1 |
| G: -6289.12860 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.54633 HOMO: -7.29809 LUMO: 2.83543 factor:1 | 1 (-2.05204) | 1 | -1 |
| G: -6289.12860 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.49572 HOMO: -6.86543 LUMO: -0.70205 factor:1 | 1 (-2.00142) | -1 | -1 |
| G: -6289.12860 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.54122 HOMO: -7.47769 LUMO: 0.31293 factor:1 | 1 (-1.04693) | -1 | -1 |
| G: -6289.12860 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.57461 HOMO: -6.63141 LUMO: -0.55511 factor:1 | 1 (-1.08032) | -1 | -1 |
| G: -6289.12860 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.67320 HOMO: -6.68856 LUMO: -0.30205 factor:1 | 1 (-1.17891) | -1 | -1 |
| G: -6289.12860 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.86651 HOMO: -7.22190 LUMO: 0.53334 factor:1 | 1 (-1.37222) | -1 | -1 |
| G: -6289.12860 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.87571 HOMO: -6.66407 LUMO: -0.27756 factor:1 | 1 (-1.38141) | -1 | -1 |
| G: -6289.12860 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.81622 HOMO: -7.15659 LUMO: -0.70205 factor:1 | 1 (-1.32193) | -1 | -1 |
| G: -6289.12860 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.97568 HOMO: -6.69400 LUMO: 1.67622 factor:1 | 1 (-1.48139) | -1 | -1 |
| G: -6289.12860 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.78226 HOMO: -6.60420 LUMO: 2.16058 factor:1 | 1 (-1.28797) | -1 | -1 |
| G: -6289.12860 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.38744 HOMO: -6.87087 LUMO: 1.88031 factor:1 | 1 (-1.89315) | -1 | -1 |
| G: -6289.12860 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.52130 HOMO: -6.60965 LUMO: -0.19864 factor:1 | 1 (-2.02700) | -1 | -1 |
| G: -6289.12860 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.29925 HOMO: -7.29265 LUMO: 0.52246 factor:1 | 1 (-1.80496) | -1 | -1 |
| G: -6289.12860 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.67130 HOMO: -6.86543 LUMO: -0.59593 factor:1 | 1 (-1.17700) | -1 | -1 |
| G: -6289.12860 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.65012 HOMO: -7.44504 LUMO: -1.01226 factor:1 | 1 (-1.15583) | -1 | -1 |
| G: -6289.12860 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.82164 HOMO: -6.92530 LUMO: -0.75103 factor:1 | 1 (-1.32734) | -1 | -1 |
| G: -6289.12860 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.69924 HOMO: -7.10489 LUMO: 2.20412 factor:1 | 1 (-1.20495) | 1 | 1 |
| G: -6289.12860 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.75658 HOMO: -6.58788 LUMO: 1.73881 factor:1 | 1 (-1.26228) | -1 | -1 |
| G: -6289.12860 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.69048 HOMO: -6.64502 LUMO: 1.70343 factor:1 | 1 (-1.19619) | -1 | -1 |
| G: -6289.12860 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.39765 HOMO: -6.73754 LUMO: 1.60819 factor:1 | 1 (-1.90335) | -1 | -1 |
| G: -6289.12860 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.60682 HOMO: -6.80829 LUMO: 2.45991 factor:1 | 1 (-2.11253) | -1 | -1 |
| G: -6289.12860 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.54734 HOMO: -6.91713 LUMO: 2.43814 factor:1 | 1 (-2.05304) | -1 | -1 |
| G: -6289.12860 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.77078 HOMO: -6.60692 LUMO: 1.93745 factor:1 | 1 (-1.27649) | -1 | -1 |
| G: -6289.12860 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.25792 HOMO: -6.26134 LUMO: 1.46125 factor:1 | 1 (-1.76362) | -1 | -1 |
| G: -6289.12860 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.38347 HOMO: -7.54028 LUMO: 0.25851 factor:1 | 1 (-1.88918) | -1 | -1 |
| G: -6289.12860 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.34524 HOMO: -6.97700 LUMO: -0.73471 factor:1 | 1 (-1.85095) | -1 | -1 |
| G: -6289.12860 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.41803 HOMO: -6.92258 LUMO: -0.70205 factor:1 | 1 (-1.92374) | -1 | -1 |
| G: -6289.12860 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.18524 HOMO: -6.83550 LUMO: -0.56872 factor:1 | 1 (-1.69094) | -1 | -1 |
| G: -6289.12860 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.19827 HOMO: -6.72121 LUMO: 1.89663 factor:1 | 1 (-1.70398) | -1 | -1 |
| G: -6289.12860 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.47436 HOMO: -6.73482 LUMO: 1.89935 factor:1 | 1 (-1.98006) | -1 | -1 |
| G: -6289.12860 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12556.70061 HOMO: -6.61781 LUMO: 1.86670 factor:1 | 1 (-3.20632) | -1 | -1 |
| G: -6289.12860 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.93363 HOMO: -7.01782 LUMO: 2.26399 factor:1 | 1 (-2.43934) | -1 | -1 |
| G: -6289.12860 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.71648 HOMO: -7.23551 LUMO: 2.09800 factor:1 | 1 (-2.22219) | 1 | 1 |
| G: -6289.12860 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12556.07206 HOMO: -7.13483 LUMO: 2.17963 factor:1 | 1 (-2.57776) | 1 | 1 |
| G: -6289.12860 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.70281 HOMO: -6.22869 LUMO: 2.01092 factor:1 | 1 (-1.20851) | -1 | -1 |
| G: -6289.12860 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12556.21807 HOMO: -6.80285 LUMO: 2.14970 factor:1 | 1 (-2.72378) | -1 | -1 |
| G: -6289.12860 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.67232 HOMO: -7.21102 LUMO: 2.33746 factor:1 | 1 (-2.17803) | 1 | 1 |
| G: -6289.12860 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.76468 HOMO: -6.39740 LUMO: 2.59597 factor:1 | 1 (-1.27039) | -1 | -1 |
| G: -6289.12860 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.61064 HOMO: -7.07768 LUMO: 2.48168 factor:1 | 1 (-1.11635) | 1 | 1 |
| G: -6289.12860 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.39020 HOMO: -7.11306 LUMO: 0.90614 factor:1 | 1 (-0.89591) | -1 | -1 |
| G: -6289.12860 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.53635 HOMO: -6.61781 LUMO: -2.46263 factor:1 | 1 (-1.04206) | -1 | -1 |
| G: -6289.12860 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.68678 HOMO: -6.96611 LUMO: 0.90614 factor:1 | 1 (-1.19248) | -1 | -1 |
| G: -6289.12860 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.26336 HOMO: -6.86271 LUMO: -1.14832 factor:1 | 1 (-1.76907) | -1 | -1 |
| G: -6289.12860 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.31811 HOMO: -6.72665 LUMO: 0.96873 factor:1 | 1 (-1.82382) | -1 | -1 |
| G: -6289.12860 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.49142 HOMO: -7.14571 LUMO: 1.05036 factor:1 | 1 (-1.99713) | -1 | -1 |
| G: -6289.12860 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.65447 HOMO: -7.14299 LUMO: 0.98777 factor:1 | 1 (-2.16018) | -1 | -1 |
| G: -6289.12860 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.40562 HOMO: -6.99333 LUMO: 1.05852 factor:1 | 1 (-1.91133) | -1 | -1 |
| G: -6289.12860 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.35355 HOMO: -6.78924 LUMO: -1.49935 factor:1 | 1 (-0.85925) | -1 | -1 |
| G: -6289.12860 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.34291 HOMO: -7.13755 LUMO: 0.94151 factor:1 | 1 (-0.84861) | -1 | -1 |
| G: -6289.12860 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12556.55971 HOMO: -6.72938 LUMO: -0.35375 factor:1 | 1 (-3.06542) | -1 | -1 |
| G: -6289.12860 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.65673 HOMO: -6.99061 LUMO: 0.82450 factor:1 | 1 (-2.16243) | -1 | -1 |
| G: -6289.12860 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.31529 HOMO: -6.75114 LUMO: -0.68028 factor:1 | 1 (-0.82099) | -1 | -1 |
| G: -6289.12860 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.92762 HOMO: -6.40556 LUMO: -0.42722 factor:1 | 1 (-2.43332) | -1 | -1 |
| G: -6289.12860 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12556.04014 HOMO: -7.18653 LUMO: 0.42178 factor:1 | 1 (-2.54584) | -1 | -1 |
| G: -6289.12860 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.26508 HOMO: -6.63958 LUMO: -0.71294 factor:1 | 1 (-1.77078) | -1 | -1 |
| G: -6289.12860 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.28399 HOMO: -6.63958 LUMO: -0.71022 factor:1 | 1 (-1.78969) | -1 | -1 |
| G: -6289.12860 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.66449 HOMO: -6.69672 LUMO: -0.72654 factor:1 | 1 (-1.17020) | -1 | -1 |
| G: -6289.12860 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.76854 HOMO: -6.56883 LUMO: -0.80274 factor:1 | 1 (-2.27425) | -1 | -1 |
| G: -6289.12860 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.67120 HOMO: -6.68584 LUMO: -0.56872 factor:1 | 1 (-2.17691) | -1 | -1 |
| G: -6289.12860 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12556.20950 HOMO: -6.59060 LUMO: -0.35647 factor:1 | 1 (-2.71521) | -1 | -1 |
| G: -6289.12860 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.89138 HOMO: -6.72121 LUMO: -0.71838 factor:1 | 1 (-1.39709) | -1 | -1 |
| G: -6289.12860 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.41596 HOMO: -6.57971 LUMO: -0.61498 factor:1 | 1 (-1.92167) | -1 | -1 |
| G: -6289.12860 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.24475 HOMO: -7.07496 LUMO: 0.50613 factor:1 | 1 (-1.75045) | -1 | -1 |
| G: -6289.12860 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.00872 HOMO: -7.14027 LUMO: 0.43266 factor:1 | 1 (-1.51442) | -1 | -1 |
| G: -6289.12860 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.95936 HOMO: -6.43277 LUMO: -0.44082 factor:1 | 1 (-1.46506) | -1 | -1 |
| G: -6289.12860 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.92877 HOMO: -6.79468 LUMO: 0.07619 factor:1 | 1 (-1.43448) | -1 | -1 |
| G: -6289.12860 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.12213 HOMO: -6.81917 LUMO: -2.57148 factor:1 | 1 (-1.62784) | -1 | -1 |
| G: -6289.12860 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.97280 HOMO: -6.71849 LUMO: 1.30615 factor:1 | 1 (-1.47850) | -1 | -1 |
| G: -6289.12860 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.79601 HOMO: -6.85455 LUMO: -0.63675 factor:1 | 1 (-1.30171) | -1 | -1 |
| G: -6289.12860 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.84499 HOMO: -6.73210 LUMO: -1.03131 factor:1 | 1 (-1.35069) | -1 | -1 |
| G: -6289.12860 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.54622 HOMO: -6.83550 LUMO: -0.58777 factor:1 | 1 (-2.05193) | -1 | -1 |
| G: -6289.12860 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.50007 HOMO: -6.53073 LUMO: -0.74287 factor:1 | 1 (-2.00578) | -1 | -1 |
| G: -6289.12860 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.36304 HOMO: -7.18381 LUMO: -0.92791 factor:1 | 1 (-1.86874) | -1 | -1 |
| G: -6289.12860 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.65281 HOMO: -6.49264 LUMO: -0.44627 factor:1 | 1 (-2.15852) | -1 | -1 |
| G: -6289.12860 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.49479 HOMO: -7.32803 LUMO: 0.41361 factor:1 | 1 (-2.00050) | -1 | -1 |
| G: -6289.12860 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.53417 HOMO: -6.53073 LUMO: -0.52790 factor:1 | 1 (-2.03987) | -1 | -1 |
| G: -6289.12860 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.63851 HOMO: -6.54978 LUMO: -0.53062 factor:1 | 1 (-1.14421) | -1 | -1 |
| G: -6289.12860 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.46551 HOMO: -6.56611 LUMO: -0.37824 factor:1 | 1 (-1.97122) | -1 | -1 |
| G: -6289.12860 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.61232 HOMO: -6.57155 LUMO: -0.64219 factor:1 | 1 (-2.11803) | -1 | -1 |
| G: -6289.12860 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.45950 HOMO: -7.08040 LUMO: 0.45715 factor:1 | 1 (-1.96521) | -1 | -1 |
| G: -6289.12860 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.42383 HOMO: -6.66679 LUMO: -0.75376 factor:1 | 1 (-1.92953) | -1 | -1 |
| G: -6289.12860 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.69110 HOMO: -6.83550 LUMO: -0.99322 factor:1 | 1 (-2.19680) | -1 | -1 |
| G: -6289.12860 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.57724 HOMO: -6.53345 LUMO: -0.29660 factor:1 | 1 (-2.08295) | -1 | -1 |
| G: -6289.12860 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.68906 HOMO: -6.65046 LUMO: 2.40549 factor:1 | 1 (-2.19476) | -1 | -1 |
| G: -6289.12860 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.50249 HOMO: -6.98788 LUMO: 2.01092 factor:1 | 1 (-2.00820) | -1 | -1 |
| G: -6289.12860 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.61806 HOMO: -6.61781 LUMO: 1.92384 factor:1 | 1 (-2.12377) | -1 | -1 |
| G: -6289.12860 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.42007 HOMO: -6.61237 LUMO: 2.06807 factor:1 | 1 (-1.92578) | -1 | -1 |
| G: -6289.12860 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.34780 HOMO: -6.59060 LUMO: 1.95106 factor:1 | 1 (-1.85350) | -1 | -1 |
| G: -6289.12860 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.72836 HOMO: -6.48175 LUMO: 1.72248 factor:1 | 1 (-1.23406) | -1 | -1 |
| G: -6289.12860 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.44113 HOMO: -6.84911 LUMO: 2.03541 factor:1 | 1 (-1.94684) | -1 | -1 |
| G: -6289.12860 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.36889 HOMO: -6.50624 LUMO: 2.17147 factor:1 | 1 (-1.87459) | -1 | -1 |
| G: -6289.12860 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.38940 HOMO: -6.68312 LUMO: 2.08439 factor:1 | 1 (-1.89511) | -1 | -1 |
| G: -6289.12860 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.48356 HOMO: -6.96067 LUMO: 1.98099 factor:1 | 1 (-1.98926) | -1 | -1 |
| G: -6289.12860 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.59907 HOMO: -6.93618 LUMO: 1.85854 factor:1 | 1 (-2.10477) | -1 | -1 |
| G: -6289.12860 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.71172 HOMO: -6.71305 LUMO: -0.61226 factor:1 | 1 (-2.21743) | -1 | -1 |
| G: -6289.12860 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.87701 HOMO: -7.06408 LUMO: 0.80001 factor:1 | 1 (-1.38272) | -1 | -1 |
| G: -6289.12860 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.32080 HOMO: -6.52257 LUMO: 0.99049 factor:1 | 1 (-1.82651) | -1 | -1 |
| G: -6289.12860 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.98714 HOMO: -6.84638 LUMO: 1.10750 factor:1 | 1 (-1.49284) | -1 | -1 |
| G: -6289.12860 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.27427 HOMO: -6.85455 LUMO: 0.84900 factor:1 | 1 (-1.77998) | -1 | -1 |
| G: -6289.12860 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.02586 HOMO: -6.60148 LUMO: -0.78369 factor:1 | 1 (-1.53157) | -1 | -1 |
| G: -6289.12860 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.39237 HOMO: -6.86543 LUMO: -0.93063 factor:1 | 1 (-1.89808) | -1 | -1 |
| G: -6289.12860 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.46897 HOMO: -6.70489 LUMO: -0.72382 factor:1 | 1 (-1.97468) | -1 | -1 |
| G: -6289.12860 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.46252 HOMO: -6.59060 LUMO: 0.31293 factor:1 | 1 (-1.96823) | -1 | -1 |
| G: -6289.12860 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.44023 HOMO: -6.52257 LUMO: -0.48708 factor:1 | 1 (-1.94594) | -1 | -1 |
| G: -6289.12860 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.04311 HOMO: -6.54706 LUMO: -0.48164 factor:1 | 1 (-1.54882) | -1 | -1 |
| G: -6289.12860 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.00779 HOMO: -7.32803 LUMO: 0.08436 factor:1 | 1 (-1.51350) | -1 | -1 |
| G: -6289.12860 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.26616 HOMO: -6.77291 LUMO: -0.66940 factor:1 | 1 (-1.77187) | -1 | -1 |
| G: -6289.12860 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.14711 HOMO: -6.68312 LUMO: -0.53062 factor:1 | 1 (-1.65282) | -1 | -1 |
| G: -6289.12860 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.10635 HOMO: -7.07768 LUMO: 0.45987 factor:1 | 1 (-1.61206) | -1 | -1 |
| G: -6289.12860 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.73323 HOMO: -6.50352 LUMO: -0.63675 factor:1 | 1 (-1.23893) | -1 | -1 |
| G: -6289.12860 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.92801 HOMO: -6.48992 LUMO: -0.60681 factor:1 | 1 (-1.43371) | -1 | -1 |
| G: -6289.12860 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.91440 HOMO: -6.65318 LUMO: -0.72382 factor:1 | 1 (-1.42011) | -1 | -1 |
| G: -6289.12860 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.85573 HOMO: -6.54706 LUMO: 0.24218 factor:1 | 1 (-1.36144) | -1 | -1 |
| G: -6289.12860 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.48422 HOMO: -6.63958 LUMO: 0.57416 factor:1 | 1 (-0.98992) | -1 | -1 |
| G: -6289.12860 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.99331 HOMO: -6.37563 LUMO: -0.48164 factor:1 | 1 (-1.49902) | -1 | -1 |
| G: -6289.12860 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.62117 HOMO: -6.64774 LUMO: -0.71838 factor:1 | 1 (-1.12688) | -1 | -1 |
| G: -6289.12860 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.35904 HOMO: -7.17020 LUMO: 0.45987 factor:1 | 1 (-1.86474) | -1 | -1 |
| G: -6289.12860 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.89507 HOMO: -6.86543 LUMO: -1.05036 factor:1 | 1 (-2.40078) | -1 | -1 |
| G: -6289.12860 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.85657 HOMO: -6.77019 LUMO: -1.03131 factor:1 | 1 (-2.36227) | -1 | -1 |
| G: -6289.12860 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12556.42352 HOMO: -6.80285 LUMO: 1.05852 factor:1 | 1 (-2.92922) | -1 | -1 |
| G: -6289.12860 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12556.25546 HOMO: -6.76475 LUMO: 1.01771 factor:1 | 1 (-2.76117) | -1 | -1 |
| G: -6289.12860 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.93594 HOMO: -6.92530 LUMO: 1.37417 factor:1 | 1 (-2.44165) | -1 | -1 |
| G: -6289.12860 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.54247 HOMO: -6.98244 LUMO: 1.25989 factor:1 | 1 (-2.04817) | -1 | -1 |
| G: -6289.12860 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.85921 HOMO: -6.74842 LUMO: 0.89798 factor:1 | 1 (-2.36491) | -1 | -1 |
| G: -6289.12860 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.81126 HOMO: -6.77019 LUMO: -1.17009 factor:1 | 1 (-2.31697) | -1 | -1 |
| G: -6289.12860 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12556.06357 HOMO: -6.78652 LUMO: 1.35785 factor:1 | 1 (-2.56927) | -1 | -1 |
| G: -6289.12860 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12556.39748 HOMO: -6.82734 LUMO: -0.68301 factor:1 | 1 (-2.90318) | -1 | -1 |
| G: -6289.12860 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12556.39677 HOMO: -6.48175 LUMO: -2.19052 factor:1 | 1 (-2.90248) | -1 | -1 |
| G: -6289.12860 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12556.55440 HOMO: -6.65863 LUMO: -0.77008 factor:1 | 1 (-3.06011) | -1 | -1 |
| G: -6289.12860 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.91496 HOMO: -6.44094 LUMO: -2.20956 factor:1 | 1 (-2.42067) | -1 | -1 |
| G: -6289.12860 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12556.60692 HOMO: -6.59876 LUMO: -0.57688 factor:1 | 1 (-3.11263) | -1 | -1 |
| G: -6289.12860 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12556.45731 HOMO: -6.78380 LUMO: -0.77008 factor:1 | 1 (-2.96302) | -1 | -1 |
| G: -6289.12860 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.65442 HOMO: -7.30354 LUMO: 0.25034 factor:1 | 1 (-2.16012) | -1 | -1 |
| G: -6289.12860 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.88794 HOMO: -6.59332 LUMO: -0.53334 factor:1 | 1 (-2.39365) | -1 | -1 |
| G: -6289.12860 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12556.57098 HOMO: -6.64230 LUMO: -0.55783 factor:1 | 1 (-3.07668) | -1 | -1 |
| G: -6289.12860 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12556.44131 HOMO: -7.26544 LUMO: 0.20409 factor:1 | 1 (-2.94702) | -1 | -1 |
| G: -6289.12860 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12556.10923 HOMO: -6.61237 LUMO: -0.65307 factor:1 | 1 (-2.61493) | -1 | -1 |
| G: -6289.12860 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.84634 HOMO: -6.72393 LUMO: -0.65307 factor:1 | 1 (-2.35204) | -1 | -1 |
| G: -6289.12860 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.55694 HOMO: -6.29671 LUMO: -0.39729 factor:1 | 1 (-2.06265) | -1 | -1 |
| G: -6289.12860 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.41551 HOMO: -6.75387 LUMO: -0.53334 factor:1 | 1 (-0.92121) | -1 | -1 |
| G: -6289.12860 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.28005 HOMO: -6.53073 LUMO: -0.31293 factor:1 | 1 (-0.78576) | -1 | -1 |
| G: -6289.12860 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.44350 HOMO: -6.42189 LUMO: -0.59049 factor:1 | 1 (-1.94921) | -1 | -1 |
| G: -6289.12860 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.49281 HOMO: -6.41100 LUMO: -0.29933 factor:1 | 1 (-1.99851) | -1 | -1 |
| G: -6289.12860 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.68609 HOMO: -6.57427 LUMO: -0.53879 factor:1 | 1 (-2.19180) | -1 | -1 |
| G: -6289.12860 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.37958 HOMO: -7.43143 LUMO: 0.33470 factor:1 | 1 (-1.88529) | -1 | -1 |
| G: -6289.12860 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.79856 HOMO: -6.56067 LUMO: -0.50885 factor:1 | 1 (-1.30427) | -1 | -1 |
| G: -6289.12860 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.65685 HOMO: -6.65863 LUMO: -0.76464 factor:1 | 1 (-1.16255) | -1 | -1 |
| G: -6289.12860 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.57687 HOMO: -6.32665 LUMO: -0.41906 factor:1 | 1 (-1.08258) | -1 | -1 |
| G: -6289.12860 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.75309 HOMO: -6.57699 LUMO: 1.63813 factor:1 | 1 (-1.25880) | -1 | -1 |
| G: -6289.12860 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.74934 HOMO: -6.53073 LUMO: 1.71704 factor:1 | 1 (-1.25504) | -1 | -1 |
| G: -6289.12860 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.45328 HOMO: -6.86271 LUMO: 2.07351 factor:1 | 1 (-0.95898) | -1 | -1 |
| G: -6289.12860 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12556.04680 HOMO: -6.63686 LUMO: 1.78235 factor:1 | 1 (-2.55251) | -1 | -1 |
| G: -6289.12860 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12556.48874 HOMO: -6.60965 LUMO: 1.94289 factor:1 | 1 (-2.99445) | -1 | -1 |
| G: -6289.12860 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.55527 HOMO: -6.55250 LUMO: 1.89119 factor:1 | 1 (-1.06097) | -1 | -1 |
| G: -6289.12860 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.89015 HOMO: -6.50624 LUMO: 1.85582 factor:1 | 1 (-2.39585) | -1 | -1 |
| G: -6289.12860 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.23318 HOMO: -6.06814 LUMO: 1.94561 factor:1 | 1 (-1.73889) | -1 | -1 |
| G: -6289.12860 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.55499 HOMO: -6.58788 LUMO: 2.01908 factor:1 | 1 (-2.06069) | -1 | -1 |
| G: -6289.12860 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12556.12569 HOMO: -6.74026 LUMO: 0.31293 factor:1 | 1 (-2.63140) | -1 | -1 |
| G: -6289.12860 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.77570 HOMO: -6.54434 LUMO: -0.42994 factor:1 | 1 (-2.28140) | -1 | -1 |
| G: -6289.12860 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.51722 HOMO: -6.94707 LUMO: 0.42994 factor:1 | 1 (-2.02292) | -1 | -1 |
| G: -6289.12860 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.43194 HOMO: -6.98516 LUMO: 0.41361 factor:1 | 1 (-1.93764) | -1 | -1 |
| G: -6289.12860 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.58217 HOMO: -6.31304 LUMO: -0.54967 factor:1 | 1 (-2.08788) | -1 | -1 |
| G: -6289.12860 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.21248 HOMO: -6.48447 LUMO: -0.40817 factor:1 | 1 (-1.71818) | -1 | -1 |
| G: -6289.12860 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.55833 HOMO: -6.49264 LUMO: 0.29116 factor:1 | 1 (-2.06404) | -1 | -1 |
| G: -6289.12860 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.85545 HOMO: -6.48719 LUMO: -0.11973 factor:1 | 1 (-2.36116) | -1 | -1 |
| G: -6289.12860 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.42883 HOMO: -7.16204 LUMO: 0.44082 factor:1 | 1 (-1.93454) | -1 | -1 |
| G: -6289.12860 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.27749 HOMO: -6.74842 LUMO: -0.37552 factor:1 | 1 (-0.78320) | -1 | -1 |
| G: -6289.12860 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.46408 HOMO: -6.44638 LUMO: -0.45171 factor:1 | 1 (-0.96979) | -1 | -1 |
| G: -6289.12860 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12553.99694 HOMO: -7.07496 LUMO: 0.50341 factor:1 | 1 (-0.50265) | -1 | -1 |
| G: -6289.12860 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.56631 HOMO: -6.79468 LUMO: 0.11429 factor:1 | 1 (-1.07202) | -1 | -1 |
| G: -6289.12860 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.33210 HOMO: -6.63958 LUMO: -0.67484 factor:1 | 1 (-1.83780) | -1 | -1 |
| G: -6289.12860 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.94101 HOMO: -7.08584 LUMO: 0.46259 factor:1 | 1 (-2.44671) | -1 | -1 |
| G: -6289.12860 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.48211 HOMO: -6.80285 LUMO: -0.73199 factor:1 | 1 (-1.98782) | -1 | -1 |
| G: -6289.12860 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.18861 HOMO: -6.44366 LUMO: -0.45443 factor:1 | 1 (-1.69432) | -1 | -1 |
| G: -6289.12860 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.86854 HOMO: -6.75931 LUMO: 0.25851 factor:1 | 1 (-2.37425) | -1 | -1 |
| G: -6289.12860 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.79665 HOMO: -6.64502 LUMO: 1.79323 factor:1 | 1 (-2.30236) | -1 | -1 |
| G: -6289.12860 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.95600 HOMO: -6.51168 LUMO: 1.60275 factor:1 | 1 (-2.46171) | -1 | -1 |
| G: -6289.12860 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.59431 HOMO: -6.56067 LUMO: 1.63268 factor:1 | 1 (-2.10001) | -1 | -1 |
| G: -6289.12860 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.42780 HOMO: -6.56883 LUMO: 1.70615 factor:1 | 1 (-1.93351) | -1 | -1 |
| G: -6289.12860 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.37030 HOMO: -6.77836 LUMO: 1.77962 factor:1 | 1 (-1.87601) | -1 | -1 |
| G: -6289.12860 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.71711 HOMO: -6.38923 LUMO: 1.85854 factor:1 | 1 (-2.22282) | -1 | -1 |
| G: -6289.12860 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.42543 HOMO: -6.35658 LUMO: 2.16875 factor:1 | 1 (-1.93114) | -1 | -1 |
| G: -6289.12860 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.78242 HOMO: -6.83006 LUMO: 2.31025 factor:1 | 1 (-2.28812) | -1 | -1 |
| G: -6289.12860 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.82971 HOMO: -6.87087 LUMO: 1.79051 factor:1 | 1 (-2.33542) | -1 | -1 |
| G: -6289.12860 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.97521 HOMO: -6.56339 LUMO: 2.37828 factor:1 | 1 (-2.48092) | -1 | -1 |
| G: -6289.12860 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.66103 HOMO: -6.30488 LUMO: 2.51705 factor:1 | 1 (-2.16673) | -1 | -1 |
| G: -6289.12860 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.51219 HOMO: -6.69400 LUMO: 1.95650 factor:1 | 1 (-1.01790) | -1 | -1 |
| G: -6289.12860 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.43222 HOMO: -6.51168 LUMO: 2.03541 factor:1 | 1 (-0.93792) | -1 | -1 |
| G: -6289.12860 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.61187 HOMO: -6.30760 LUMO: 1.65173 factor:1 | 1 (-1.11757) | -1 | -1 |
| G: -6289.12860 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.32040 HOMO: -6.55250 LUMO: 1.90752 factor:1 | 1 (-0.82611) | -1 | -1 |
| G: -6289.12860 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.59978 HOMO: -6.41372 LUMO: 1.76058 factor:1 | 1 (-1.10549) | -1 | -1 |
| G: -6289.12860 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.40179 HOMO: -6.23957 LUMO: 2.06534 factor:1 | 1 (-1.90749) | -1 | -1 |
| G: -6289.12860 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.97271 HOMO: -6.58243 LUMO: 2.11705 factor:1 | 1 (-2.47841) | -1 | -1 |
| G: -6289.12860 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.34627 HOMO: -6.37835 LUMO: 2.09256 factor:1 | 1 (-1.85198) | -1 | -1 |
| G: -6289.12860 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12556.20109 HOMO: -6.50624 LUMO: 2.55787 factor:1 | 1 (-2.70680) | -1 | -1 |
| G: -6289.12860 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.54625 HOMO: -6.45454 LUMO: 1.87214 factor:1 | 1 (-2.05196) | -1 | -1 |
| G: -6289.12860 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.88593 HOMO: -6.53617 LUMO: 1.95650 factor:1 | 1 (-2.39164) | -1 | -1 |
| G: -6289.12860 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.32987 HOMO: -6.51985 LUMO: 1.71432 factor:1 | 1 (-1.83557) | -1 | -1 |
| G: -6289.12860 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.18616 HOMO: -6.75114 LUMO: 1.84493 factor:1 | 1 (-1.69187) | -1 | -1 |
| G: -6289.12860 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.41874 HOMO: -6.06270 LUMO: 1.65717 factor:1 | 1 (-1.92444) | -1 | -1 |
| G: -6289.12860 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.47463 HOMO: -5.89671 LUMO: 1.71704 factor:1 | 1 (-1.98034) | -1 | -1 |
| G: -6289.12860 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.20216 HOMO: -6.18787 LUMO: 1.91840 factor:1 | 1 (-1.70787) | -1 | -1 |
| G: -6289.12860 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.10755 HOMO: -6.01644 LUMO: 1.85582 factor:1 | 1 (-1.61325) | -1 | -1 |
| G: -6289.12860 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.89584 HOMO: -6.05998 LUMO: 2.33474 factor:1 | 1 (-1.40155) | -1 | -1 |
| G: -6289.12860 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.05076 HOMO: -6.05725 LUMO: 2.03541 factor:1 | 1 (-1.55646) | -1 | -1 |
| G: -6289.12860 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.35009 HOMO: -6.80829 LUMO: 1.90480 factor:1 | 1 (-0.85580) | -1 | -1 |
| G: -6289.12860 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.53429 HOMO: -6.76475 LUMO: 2.20956 factor:1 | 1 (-1.03999) | -1 | -1 |
| G: -6289.12860 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.68240 HOMO: -6.29944 LUMO: 1.77962 factor:1 | 1 (-1.18810) | -1 | -1 |
| G: -6289.12860 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.84537 HOMO: -6.47359 LUMO: -0.25579 factor:1 | 1 (-1.35107) | -1 | -1 |
| G: -6289.12860 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.72025 HOMO: -6.57699 LUMO: -0.47348 factor:1 | 1 (-1.22595) | -1 | -1 |
| G: -6289.12860 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.33523 HOMO: -7.20830 LUMO: 0.49797 factor:1 | 1 (-0.84094) | -1 | -1 |
| G: -6289.12860 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.41393 HOMO: -7.49402 LUMO: 0.29933 factor:1 | 1 (-0.91964) | -1 | -1 |
| G: -6289.12860 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.74822 HOMO: -6.66679 LUMO: -0.58777 factor:1 | 1 (-1.25393) | -1 | -1 |
| G: -6289.12860 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.38854 HOMO: -6.67767 LUMO: -0.56328 factor:1 | 1 (-0.89425) | -1 | -1 |
| G: -6289.12860 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.62724 HOMO: -7.42871 LUMO: 0.35647 factor:1 | 1 (-1.13295) | -1 | -1 |
| G: -6289.12860 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.29366 HOMO: -6.56067 LUMO: -0.54423 factor:1 | 1 (-0.79936) | -1 | -1 |
| G: -6289.12860 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.77864 HOMO: -6.56339 LUMO: -0.50341 factor:1 | 1 (-1.28435) | -1 | -1 |
| G: -6289.12860 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.46397 HOMO: -6.56067 LUMO: -0.48436 factor:1 | 1 (-0.96968) | -1 | -1 |
| G: -6289.12860 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.63271 HOMO: -6.73210 LUMO: 1.75241 factor:1 | 1 (-1.13842) | -1 | -1 |
| G: -6289.12860 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.62936 HOMO: -6.48175 LUMO: 1.91296 factor:1 | 1 (-1.13507) | -1 | -1 |
| G: -6289.12860 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.30228 HOMO: -6.67767 LUMO: 1.70343 factor:1 | 1 (-0.80799) | -1 | -1 |
| G: -6289.12860 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.20144 HOMO: -6.37835 LUMO: 1.96466 factor:1 | 1 (-0.70714) | -1 | -1 |
| G: -6289.12860 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.38955 HOMO: -6.40828 LUMO: 2.10072 factor:1 | 1 (-0.89525) | -1 | -1 |
| G: -6289.12860 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.42691 HOMO: -6.06542 LUMO: 1.92112 factor:1 | 1 (-0.93262) | -1 | -1 |
| G: -6289.12860 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.53001 HOMO: -6.90353 LUMO: 1.83133 factor:1 | 1 (-1.03572) | -1 | -1 |
| G: -6289.12860 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.44019 HOMO: -6.37019 LUMO: 1.92929 factor:1 | 1 (-0.94589) | -1 | -1 |
| G: -6289.12860 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.25118 HOMO: -6.61509 LUMO: 2.11160 factor:1 | 1 (-0.75688) | -1 | -1 |
| G: -6289.12860 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.74692 HOMO: -6.82734 LUMO: 1.77146 factor:1 | 1 (-1.25262) | -1 | -1 |
| G: -6289.12860 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.66773 HOMO: -6.01100 LUMO: 1.89935 factor:1 | 1 (-1.17344) | -1 | -1 |
| G: -6289.12860 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.80055 HOMO: -6.49536 LUMO: 1.75241 factor:1 | 1 (-1.30626) | -1 | -1 |
| G: -6289.12860 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.66735 HOMO: -6.34297 LUMO: 1.86398 factor:1 | 1 (-1.17306) | -1 | -1 |
| G: -6289.12860 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.41320 HOMO: -6.53073 LUMO: 1.84493 factor:1 | 1 (-0.91890) | -1 | -1 |
| G: -6289.12860 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.52378 HOMO: -6.53345 LUMO: 2.41093 factor:1 | 1 (-1.02949) | -1 | -1 |
| G: -6289.12860 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.56373 HOMO: -7.01237 LUMO: 2.06262 factor:1 | 1 (-1.06943) | -1 | -1 |
| G: -6289.12860 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.19877 HOMO: -6.17154 LUMO: 1.89119 factor:1 | 1 (-0.70448) | -1 | -1 |
| G: -6289.12860 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.26500 HOMO: -6.08719 LUMO: 1.74425 factor:1 | 1 (-0.77071) | -1 | -1 |
| G: -6289.12860 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.42604 HOMO: -6.69672 LUMO: 1.95106 factor:1 | 1 (-0.93175) | -1 | -1 |
| G: -6289.12860 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.46571 HOMO: -6.58243 LUMO: 2.24766 factor:1 | 1 (-0.97142) | -1 | -1 |
| G: -6289.12860 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.56142 HOMO: -6.74570 LUMO: 2.02181 factor:1 | 1 (-1.06712) | -1 | -1 |
| G: -6289.12860 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.54381 HOMO: -6.53890 LUMO: 1.92929 factor:1 | 1 (-1.04952) | -1 | -1 |
| G: -6289.12860 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.67834 HOMO: -6.03276 LUMO: 1.67078 factor:1 | 1 (-1.18405) | -1 | -1 |
| G: -6289.12860 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.42332 HOMO: -6.67767 LUMO: 2.03541 factor:1 | 1 (-0.92902) | -1 | -1 |
| G: -6289.12860 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.46095 HOMO: -5.98378 LUMO: 1.84221 factor:1 | 1 (-0.96666) | -1 | -1 |
| G: -6289.12860 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.10170 HOMO: -6.07086 LUMO: 2.01908 factor:1 | 1 (-1.60740) | -1 | -1 |
| G: -6289.12860 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.20706 HOMO: -6.29944 LUMO: 1.90208 factor:1 | 1 (-1.71277) | -1 | -1 |
| G: -6289.12860 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.30053 HOMO: -6.75114 LUMO: 1.85854 factor:1 | 1 (-1.80624) | -1 | -1 |
| G: -6289.12860 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.34951 HOMO: -6.56611 LUMO: 2.49801 factor:1 | 1 (-1.85522) | -1 | -1 |
| G: -6289.12860 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.98787 HOMO: -6.39740 LUMO: 1.92929 factor:1 | 1 (-1.49358) | -1 | -1 |
| G: -6289.12860 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.99492 HOMO: -6.85999 LUMO: -1.07757 factor:1 | 1 (-1.50063) | -1 | -1 |
| G: -6289.12860 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.35988 HOMO: -6.98244 LUMO: 1.07213 factor:1 | 1 (-1.86559) | -1 | -1 |
| G: -6289.12860 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.15843 HOMO: -7.04231 LUMO: 0.64219 factor:1 | 1 (-1.66414) | -1 | -1 |
| G: -6289.12860 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.70421 HOMO: -6.96339 LUMO: 0.75648 factor:1 | 1 (-2.20992) | -1 | -1 |
| G: -6289.12860 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.80133 HOMO: -6.83822 LUMO: -0.97417 factor:1 | 1 (-2.30704) | -1 | -1 |
| G: -6289.12860 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12556.57601 HOMO: -6.44910 LUMO: -2.15242 factor:1 | 1 (-3.08172) | -1 | -1 |
| G: -6289.12860 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12556.55519 HOMO: -6.84094 LUMO: -1.37690 factor:1 | 1 (-3.06090) | -1 | -1 |
| G: -6289.12860 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.83722 HOMO: -6.74026 LUMO: -2.54699 factor:1 | 1 (-2.34293) | -1 | -1 |
| G: -6289.12860 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12556.40556 HOMO: -6.96611 LUMO: 1.24900 factor:1 | 1 (-2.91126) | -1 | -1 |
| G: -6289.12860 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12556.27206 HOMO: -7.21102 LUMO: 0.82995 factor:1 | 1 (-2.77777) | -1 | -1 |
| G: -6289.12860 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.60386 HOMO: -6.88448 LUMO: 0.81634 factor:1 | 1 (-2.10956) | -1 | -1 |
| G: -6289.12860 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12556.09045 HOMO: -7.04231 LUMO: 1.10750 factor:1 | 1 (-2.59616) | -1 | -1 |
| G: -6289.12860 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.45866 HOMO: -6.83550 LUMO: -0.98777 factor:1 | 1 (-1.96436) | -1 | -1 |
| G: -6289.12860 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.46579 HOMO: -6.82189 LUMO: 0.93879 factor:1 | 1 (-1.97149) | -1 | -1 |
| G: -6289.12860 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.36274 HOMO: -6.81101 LUMO: 0.70750 factor:1 | 1 (-1.86844) | -1 | -1 |
| G: -6289.12860 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.71178 HOMO: -7.06680 LUMO: 0.74015 factor:1 | 1 (-2.21748) | -1 | -1 |
| G: -6289.12860 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.39857 HOMO: -6.68856 LUMO: 0.86260 factor:1 | 1 (-1.90428) | -1 | -1 |
| G: -6289.12860 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.61440 HOMO: -6.83822 LUMO: -0.63403 factor:1 | 1 (-1.12010) | -1 | -1 |
| G: -6289.12860 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.61851 HOMO: -6.84911 LUMO: 1.26533 factor:1 | 1 (-1.12421) | -1 | -1 |
| G: -6289.12860 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.30334 HOMO: -7.01237 LUMO: 0.73743 factor:1 | 1 (-0.80905) | -1 | -1 |
| G: -6289.12860 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.71309 HOMO: -7.00965 LUMO: 1.40139 factor:1 | 1 (-1.21880) | -1 | -1 |
| G: -6289.12860 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.50000 HOMO: -6.73210 LUMO: -2.49256 factor:1 | 1 (-1.00571) | -1 | -1 |
| G: -6289.12860 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.29050 HOMO: -7.08040 LUMO: 0.84627 factor:1 | 1 (-0.79621) | -1 | -1 |
| G: -6289.12860 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.54531 HOMO: -7.00965 LUMO: 0.82995 factor:1 | 1 (-1.05101) | -1 | -1 |
| G: -6289.12860 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.39230 HOMO: -6.88448 LUMO: 0.82723 factor:1 | 1 (-0.89800) | -1 | -1 |
| G: -6289.12860 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.87047 HOMO: -7.20013 LUMO: 0.88437 factor:1 | 1 (-2.37618) | -1 | -1 |
| G: -6289.12860 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12556.40550 HOMO: -6.60420 LUMO: -0.53334 factor:1 | 1 (-2.91121) | -1 | -1 |
| G: -6289.12860 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.53828 HOMO: -6.78652 LUMO: -0.79729 factor:1 | 1 (-2.04398) | -1 | -1 |
| G: -6289.12860 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12556.52069 HOMO: -6.48992 LUMO: -0.64491 factor:1 | 1 (-3.02640) | -1 | -1 |
| G: -6289.12860 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12556.22874 HOMO: -6.85999 LUMO: -0.78097 factor:1 | 1 (-2.73444) | -1 | -1 |
| G: -6289.12860 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.26968 HOMO: -6.65046 LUMO: -0.78097 factor:1 | 1 (-0.77539) | -1 | -1 |
| G: -6289.12860 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.48653 HOMO: -7.24095 LUMO: 0.37280 factor:1 | 1 (-0.99224) | -1 | -1 |
| G: -6289.12860 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.27308 HOMO: -6.81101 LUMO: -0.74831 factor:1 | 1 (-0.77879) | -1 | -1 |
| G: -6289.12860 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.87967 HOMO: -6.69400 LUMO: -0.77280 factor:1 | 1 (-2.38538) | -1 | -1 |
| G: -6289.12860 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.10967 HOMO: -6.08447 LUMO: -0.68573 factor:1 | 1 (-1.61538) | -1 | -1 |
| G: -6289.12860 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.28453 HOMO: -6.66679 LUMO: -0.47076 factor:1 | 1 (-1.79024) | -1 | -1 |
| G: -6289.12860 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12556.05744 HOMO: -6.97428 LUMO: -1.10750 factor:1 | 1 (-2.56315) | -1 | -1 |
| G: -6289.12860 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.19008 HOMO: -6.69128 LUMO: -0.54151 factor:1 | 1 (-1.69579) | -1 | -1 |
| G: -6289.12860 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.80177 HOMO: -6.53617 LUMO: -0.35375 factor:1 | 1 (-2.30747) | -1 | -1 |
| G: -6289.12860 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.96692 HOMO: -6.75659 LUMO: -0.41361 factor:1 | 1 (-1.47263) | -1 | -1 |
| G: -6289.12860 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.46219 HOMO: -6.69400 LUMO: -0.67484 factor:1 | 1 (-1.96790) | -1 | -1 |
| G: -6289.12860 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.51469 HOMO: -6.89264 LUMO: -0.90886 factor:1 | 1 (-2.02039) | -1 | -1 |
| G: -6289.12860 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.28654 HOMO: -6.56339 LUMO: -0.52518 factor:1 | 1 (-1.79225) | -1 | -1 |
| G: -6289.12860 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.33955 HOMO: -6.45726 LUMO: -0.65852 factor:1 | 1 (-1.84526) | -1 | -1 |
| G: -6289.12860 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.43308 HOMO: -6.80557 LUMO: -0.56600 factor:1 | 1 (-1.93878) | -1 | -1 |
| G: -6289.12860 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.27237 HOMO: -7.19469 LUMO: -0.91702 factor:1 | 1 (-1.77807) | -1 | -1 |
| G: -6289.12860 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.29114 HOMO: -6.41100 LUMO: 0.79185 factor:1 | 1 (-1.79685) | -1 | -1 |
| G: -6289.12860 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.09334 HOMO: -6.39195 LUMO: 0.26123 factor:1 | 1 (-1.59905) | -1 | -1 |
| G: -6289.12860 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.70125 HOMO: -6.78924 LUMO: 0.35919 factor:1 | 1 (-2.20695) | -1 | -1 |
| G: -6289.12860 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.47221 HOMO: -6.50624 LUMO: 0.71838 factor:1 | 1 (-1.97791) | -1 | -1 |
| G: -6289.12860 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.67575 HOMO: -6.68584 LUMO: -0.66124 factor:1 | 1 (-2.18146) | -1 | -1 |
| G: -6289.12860 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12556.24724 HOMO: -6.45182 LUMO: -0.48980 factor:1 | 1 (-2.75295) | -1 | -1 |
| G: -6289.12860 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.42998 HOMO: -7.18925 LUMO: -1.01498 factor:1 | 1 (-1.93568) | -1 | -1 |
| G: -6289.12860 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12556.02416 HOMO: -7.18925 LUMO: -0.63130 factor:1 | 1 (-2.52987) | -1 | -1 |
| G: -6289.12860 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.28502 HOMO: -6.66679 LUMO: -0.57960 factor:1 | 1 (-1.79073) | -1 | -1 |
| G: -6289.12860 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.44636 HOMO: -6.44910 LUMO: -0.30205 factor:1 | 1 (-1.95206) | -1 | -1 |
| G: -6289.12860 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.29955 HOMO: -7.23279 LUMO: 0.46804 factor:1 | 1 (-1.80526) | -1 | -1 |
| G: -6289.12860 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.13996 HOMO: -6.92802 LUMO: -0.72927 factor:1 | 1 (-1.64566) | -1 | -1 |
| G: -6289.12860 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.45069 HOMO: -6.83278 LUMO: -0.59321 factor:1 | 1 (-0.95640) | -1 | -1 |
| G: -6289.12860 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.28729 HOMO: -7.44776 LUMO: 0.27211 factor:1 | 1 (-0.79299) | -1 | -1 |
| G: -6289.12860 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.28609 HOMO: -6.80829 LUMO: -0.59865 factor:1 | 1 (-0.79180) | -1 | -1 |
| G: -6289.12860 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.41619 HOMO: -6.63686 LUMO: -0.75103 factor:1 | 1 (-0.92189) | -1 | -1 |
| G: -6289.12860 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.45989 HOMO: -6.73210 LUMO: -0.55511 factor:1 | 1 (-0.96560) | -1 | -1 |
| G: -6289.12860 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.17227 HOMO: -6.50624 LUMO: 1.58642 factor:1 | 1 (-0.67797) | -1 | -1 |
| G: -6289.12860 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.18378 HOMO: -6.79196 LUMO: 0.96328 factor:1 | 1 (-0.68948) | -1 | -1 |
| G: -6289.12860 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.42408 HOMO: -6.82734 LUMO: 1.23540 factor:1 | 1 (-0.92979) | -1 | -1 |
| G: -6289.12860 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.23956 HOMO: -6.90081 LUMO: 1.25444 factor:1 | 1 (-0.74527) | -1 | -1 |
| G: -6289.12860 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.01452 HOMO: -7.00965 LUMO: -1.05036 factor:1 | 1 (-0.52023) | -1 | -1 |
| G: -6289.12860 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.36002 HOMO: -7.01237 LUMO: -1.48302 factor:1 | 1 (-0.86573) | -1 | -1 |
| G: -6289.12860 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.24974 HOMO: -6.91713 LUMO: 0.93607 factor:1 | 1 (-0.75544) | -1 | -1 |
| G: -6289.12860 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.69458 HOMO: -7.02598 LUMO: 0.92247 factor:1 | 1 (-2.20029) | -1 | -1 |
| G: -6289.12860 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12556.54091 HOMO: -6.98516 LUMO: 1.52384 factor:1 | 1 (-3.04661) | -1 | -1 |
| G: -6289.12860 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.47561 HOMO: -6.75387 LUMO: 1.04764 factor:1 | 1 (-1.98132) | -1 | -1 |
| G: -6289.12860 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.17578 HOMO: -7.09401 LUMO: 1.19458 factor:1 | 1 (-0.68148) | -1 | -1 |
| G: -6289.12860 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.32821 HOMO: -6.88992 LUMO: -1.56193 factor:1 | 1 (-0.83392) | -1 | -1 |
| G: -6289.12860 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.30291 HOMO: -7.00149 LUMO: 0.99866 factor:1 | 1 (-0.80861) | -1 | -1 |
| G: -6289.12860 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.90936 HOMO: -7.13755 LUMO: 1.05308 factor:1 | 1 (-2.41506) | -1 | -1 |
| G: -6289.12860 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.22799 HOMO: -6.85183 LUMO: -1.42860 factor:1 | 1 (-1.73369) | -1 | -1 |
| G: -6289.12860 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.76027 HOMO: -6.63141 LUMO: -0.88981 factor:1 | 1 (-2.26597) | -1 | -1 |
| G: -6289.12860 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.15008 HOMO: -6.92258 LUMO: -0.82178 factor:1 | 1 (-1.65579) | -1 | -1 |
| G: -6289.12860 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.30859 HOMO: -6.55794 LUMO: -0.80818 factor:1 | 1 (-1.81429) | -1 | -1 |
| G: -6289.12860 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12556.02985 HOMO: -6.95251 LUMO: -0.97145 factor:1 | 1 (-2.53556) | -1 | -1 |
| G: -6289.12860 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.39613 HOMO: -7.37701 LUMO: 0.14150 factor:1 | 1 (-1.90183) | -1 | -1 |
| G: -6289.12860 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12556.18607 HOMO: -6.74842 LUMO: -0.68028 factor:1 | 1 (-2.69178) | -1 | -1 |
| G: -6289.12860 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.23756 HOMO: -6.65046 LUMO: -0.52518 factor:1 | 1 (-1.74327) | -1 | -1 |
| G: -6289.12860 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.66379 HOMO: -6.91441 LUMO: -1.13199 factor:1 | 1 (-1.16949) | -1 | -1 |
| G: -6289.12860 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.52811 HOMO: -7.00965 LUMO: -1.00682 factor:1 | 1 (-1.03381) | -1 | -1 |
| G: -6289.12860 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.71554 HOMO: -6.55794 LUMO: -0.54967 factor:1 | 1 (-1.22125) | -1 | -1 |
| G: -6289.12860 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.53162 HOMO: -6.71577 LUMO: -0.53879 factor:1 | 1 (-1.03733) | -1 | -1 |
| G: -6289.12860 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.36748 HOMO: -6.88992 LUMO: -0.55511 factor:1 | 1 (-0.87319) | -1 | -1 |
| G: -6289.12860 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.70226 HOMO: -6.74026 LUMO: -0.60681 factor:1 | 1 (-1.20797) | -1 | -1 |
| G: -6289.12860 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.97987 HOMO: -6.76747 LUMO: -0.50885 factor:1 | 1 (-1.48558) | -1 | -1 |
| G: -6289.12860 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.93024 HOMO: -6.87904 LUMO: -0.92519 factor:1 | 1 (-1.43594) | -1 | -1 |
| G: -6289.12860 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.80942 HOMO: -6.53073 LUMO: -0.53062 factor:1 | 1 (-1.31513) | -1 | -1 |
| G: -6289.12860 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.43570 HOMO: -6.97700 LUMO: -0.98505 factor:1 | 1 (-0.94141) | -1 | -1 |
| G: -6289.12860 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.96667 HOMO: -6.96884 LUMO: -0.79185 factor:1 | 1 (-1.47238) | -1 | -1 |
| G: -6289.12860 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.70354 HOMO: -6.60420 LUMO: -0.31021 factor:1 | 1 (-1.20925) | -1 | -1 |
| G: -6289.12860 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.84681 HOMO: -6.68584 LUMO: -0.63947 factor:1 | 1 (-1.35251) | -1 | -1 |
| G: -6289.12860 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.75056 HOMO: -6.41917 LUMO: -0.35103 factor:1 | 1 (-1.25627) | -1 | -1 |
| G: -6289.12860 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.85497 HOMO: -6.73482 LUMO: -0.70477 factor:1 | 1 (-1.36068) | -1 | -1 |
| G: -6289.12860 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.87220 HOMO: -6.71305 LUMO: -0.85716 factor:1 | 1 (-1.37790) | -1 | -1 |
| G: -6289.12860 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.69236 HOMO: -6.70761 LUMO: -0.63403 factor:1 | 1 (-1.19806) | -1 | -1 |
| G: -6289.12860 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.53344 HOMO: -6.37563 LUMO: -0.38640 factor:1 | 1 (-1.03915) | -1 | -1 |
| G: -6289.12860 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.70104 HOMO: -6.27495 LUMO: -0.54967 factor:1 | 1 (-1.20674) | -1 | -1 |
| G: -6289.12860 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.68400 HOMO: -6.98516 LUMO: 0.38096 factor:1 | 1 (-1.18971) | -1 | -1 |
| G: -6289.12860 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.37143 HOMO: -6.47087 LUMO: -0.40001 factor:1 | 1 (-0.87713) | -1 | -1 |
| G: -6289.12860 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.71546 HOMO: -6.59876 LUMO: 0.20681 factor:1 | 1 (-1.22117) | -1 | -1 |
| G: -6289.12860 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.74888 HOMO: -6.89809 LUMO: 0.14966 factor:1 | 1 (-1.25458) | -1 | -1 |
| G: -6289.12860 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.37329 HOMO: -6.76203 LUMO: 2.11432 factor:1 | 1 (-1.87900) | -1 | -1 |
| G: -6289.12860 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.41319 HOMO: -6.58516 LUMO: 1.75786 factor:1 | 1 (-1.91889) | -1 | -1 |
| G: -6289.12860 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.61496 HOMO: -6.37835 LUMO: 1.84493 factor:1 | 1 (-2.12066) | -1 | -1 |
| G: -6289.12860 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.59529 HOMO: -6.83550 LUMO: 1.74425 factor:1 | 1 (-2.10099) | -1 | -1 |
| G: -6289.12860 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.52426 HOMO: -6.65318 LUMO: 1.79051 factor:1 | 1 (-2.02997) | -1 | -1 |
| G: -6289.12860 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.46176 HOMO: -6.68584 LUMO: 2.11160 factor:1 | 1 (-1.96746) | -1 | -1 |
| G: -6289.12860 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.80063 HOMO: -6.36202 LUMO: 1.85037 factor:1 | 1 (-1.30634) | -1 | -1 |
| G: -6289.12860 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.93165 HOMO: -6.68312 LUMO: 2.23133 factor:1 | 1 (-1.43736) | -1 | -1 |
| G: -6289.12860 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.79171 HOMO: -6.66679 LUMO: 2.14154 factor:1 | 1 (-1.29741) | -1 | -1 |
| G: -6289.12860 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.04488 HOMO: -6.50896 LUMO: 1.92657 factor:1 | 1 (-1.55059) | -1 | -1 |
| G: -6289.12860 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.32366 HOMO: -6.63686 LUMO: 2.22317 factor:1 | 1 (-1.82937) | -1 | -1 |
| G: -6289.12860 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.24480 HOMO: -6.58788 LUMO: 2.17419 factor:1 | 1 (-1.75051) | -1 | -1 |
| G: -6289.12860 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.30709 HOMO: -6.72665 LUMO: 2.12249 factor:1 | 1 (-1.81280) | -1 | -1 |
| G: -6289.12860 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.36823 HOMO: -6.28311 LUMO: 1.91024 factor:1 | 1 (-1.87394) | -1 | -1 |
| G: -6289.12860 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.25479 HOMO: -6.56067 LUMO: 2.27487 factor:1 | 1 (-1.76050) | -1 | -1 |
| G: -6289.12860 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.98858 HOMO: -6.83006 LUMO: 2.28031 factor:1 | 1 (-1.49429) | -1 | -1 |
| G: -6289.12860 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.49531 HOMO: -6.45182 LUMO: 1.62724 factor:1 | 1 (-2.00102) | -1 | -1 |
| G: -6289.12860 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.42979 HOMO: -6.78380 LUMO: 1.83677 factor:1 | 1 (-1.93549) | -1 | -1 |
| G: -6289.12860 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.28491 HOMO: -6.23413 LUMO: 1.80956 factor:1 | 1 (-1.79062) | -1 | -1 |
| G: -6289.12860 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.09043 HOMO: -6.74298 LUMO: 2.16875 factor:1 | 1 (-1.59614) | -1 | -1 |
| G: -6289.12860 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.10589 HOMO: -6.81645 LUMO: 2.50073 factor:1 | 1 (-1.61159) | -1 | -1 |
| G: -6289.12860 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.33610 HOMO: -6.71033 LUMO: 1.96466 factor:1 | 1 (-1.84180) | -1 | -1 |
| G: -6289.12860 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.36807 HOMO: -6.83550 LUMO: 2.04358 factor:1 | 1 (-1.87378) | -1 | -1 |
| G: -6289.12860 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.10679 HOMO: -6.60965 LUMO: 2.38100 factor:1 | 1 (-1.61249) | -1 | -1 |
| G: -6289.12860 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.94224 HOMO: -6.73210 LUMO: 2.26127 factor:1 | 1 (-1.44795) | -1 | -1 |
| G: -6289.12860 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.29370 HOMO: -6.76203 LUMO: 2.13609 factor:1 | 1 (-1.79941) | -1 | -1 |
| G: -6289.12860 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.35142 HOMO: -6.71033 LUMO: 2.05990 factor:1 | 1 (-1.85712) | -1 | -1 |
| G: -6289.12860 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.63042 HOMO: -6.50896 LUMO: 2.32385 factor:1 | 1 (-1.13613) | -1 | -1 |
| G: -6289.12860 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.56806 HOMO: -6.53345 LUMO: 1.74425 factor:1 | 1 (-1.07376) | -1 | -1 |
| G: -6289.12860 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.39341 HOMO: -6.25862 LUMO: 1.63540 factor:1 | 1 (-0.89912) | -1 | -1 |
| G: -6289.12860 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.21458 HOMO: -5.90759 LUMO: 1.78779 factor:1 | 1 (-0.72029) | -1 | -1 |
| G: -6289.12860 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.14043 HOMO: -6.09807 LUMO: 1.99732 factor:1 | 1 (-0.64613) | -1 | -1 |
| G: -6289.12860 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.77296 HOMO: -5.92392 LUMO: 1.99732 factor:1 | 1 (-1.27866) | -1 | -1 |
| G: -6289.12860 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.45850 HOMO: -6.45182 LUMO: 1.72248 factor:1 | 1 (-0.96421) | -1 | -1 |
| G: -6289.12860 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.61687 HOMO: -6.53073 LUMO: 1.82588 factor:1 | 1 (-1.12258) | -1 | -1 |
| G: -6289.12860 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.70006 HOMO: -6.40828 LUMO: 2.05174 factor:1 | 1 (-1.20576) | -1 | -1 |
| G: -6289.12860 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.50748 HOMO: -6.60420 LUMO: -0.82450 factor:1 | 1 (-1.01319) | -1 | -1 |
| G: -6289.12860 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.34389 HOMO: -6.76747 LUMO: -0.57144 factor:1 | 1 (-0.84959) | -1 | -1 |
| G: -6289.12860 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.59108 HOMO: -6.67767 LUMO: -0.59321 factor:1 | 1 (-1.09678) | -1 | -1 |
| G: -6289.12860 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.49173 HOMO: -6.65863 LUMO: -0.57416 factor:1 | 1 (-0.99743) | -1 | -1 |
| G: -6289.12860 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.62348 HOMO: -6.49808 LUMO: -0.54695 factor:1 | 1 (-1.12919) | -1 | -1 |
| G: -6289.12860 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.41907 HOMO: -6.50080 LUMO: -0.61498 factor:1 | 1 (-0.92478) | -1 | -1 |
| G: -6289.12860 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.27417 HOMO: -6.74842 LUMO: -0.51974 factor:1 | 1 (-0.77988) | -1 | -1 |
| G: -6289.12860 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.55823 HOMO: -6.13345 LUMO: 0.67756 factor:1 | 1 (-1.06394) | -1 | -1 |
| G: -6289.12860 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.24412 HOMO: -6.48719 LUMO: 0.52790 factor:1 | 1 (-1.74983) | -1 | -1 |
| G: -6289.12860 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.28050 HOMO: -6.35930 LUMO: 0.74015 factor:1 | 1 (-1.78621) | -1 | -1 |
| G: -6289.12860 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.20548 HOMO: -6.41644 LUMO: 0.22313 factor:1 | 1 (-1.71119) | -1 | -1 |
| G: -6289.12860 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.85255 HOMO: -6.85727 LUMO: -0.00272 factor:1 | 1 (-1.35826) | -1 | -1 |
| G: -6289.12860 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.27327 HOMO: -6.84638 LUMO: 0.24762 factor:1 | 1 (-1.77897) | -1 | -1 |
| G: -6289.12860 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.07533 HOMO: -6.66951 LUMO: 0.39184 factor:1 | 1 (-1.58104) | -1 | -1 |
| G: -6289.12860 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.75056 HOMO: -6.62597 LUMO: -0.65035 factor:1 | 1 (-1.25627) | -1 | -1 |
| G: -6289.12860 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.52359 HOMO: -7.13755 LUMO: 0.45715 factor:1 | 1 (-1.02930) | -1 | -1 |
| G: -6289.12860 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.60291 HOMO: -7.12666 LUMO: 0.45171 factor:1 | 1 (-1.10862) | -1 | -1 |
| G: -6289.12860 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.25371 HOMO: -6.46270 LUMO: -0.46259 factor:1 | 1 (-0.75942) | -1 | -1 |
| G: -6289.12860 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.67540 HOMO: -6.36202 LUMO: -0.29660 factor:1 | 1 (-1.18111) | -1 | -1 |
| G: -6289.12860 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.34794 HOMO: -6.28583 LUMO: 0.40545 factor:1 | 1 (-0.85365) | -1 | -1 |
| G: -6289.12860 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.19618 HOMO: -6.70761 LUMO: 0.41906 factor:1 | 1 (-0.70189) | -1 | -1 |
| G: -6289.12860 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.47156 HOMO: -6.76203 LUMO: -0.60954 factor:1 | 1 (-0.97727) | -1 | -1 |
| G: -6289.12860 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.44552 HOMO: -6.85999 LUMO: -0.75103 factor:1 | 1 (-0.95123) | -1 | -1 |
| G: -6289.12860 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.63059 HOMO: -7.19741 LUMO: -1.00954 factor:1 | 1 (-1.13629) | -1 | -1 |
| G: -6289.12860 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.74634 HOMO: -6.58243 LUMO: -0.33470 factor:1 | 1 (-1.25205) | -1 | -1 |
| G: -6289.12860 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.83247 HOMO: -7.22190 LUMO: 0.49253 factor:1 | 1 (-1.33817) | -1 | -1 |
| G: -6289.12860 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.58528 HOMO: -7.22462 LUMO: 0.51974 factor:1 | 1 (-1.09099) | -1 | -1 |
| G: -6289.12860 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.54672 HOMO: -7.08584 LUMO: -0.68301 factor:1 | 1 (-1.05243) | -1 | -1 |
| G: -6289.12860 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.42247 HOMO: -6.68584 LUMO: -0.29660 factor:1 | 1 (-0.92818) | -1 | -1 |
| G: -6289.12860 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.54158 HOMO: -6.33753 LUMO: -0.48436 factor:1 | 1 (-1.04728) | -1 | -1 |
| G: -6289.12860 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.55548 HOMO: -7.15932 LUMO: 0.55511 factor:1 | 1 (-1.06119) | -1 | -1 |
| G: -6289.12860 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.29717 HOMO: -6.57427 LUMO: 2.01908 factor:1 | 1 (-0.80287) | -1 | -1 |
| G: -6289.12860 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.61508 HOMO: -6.75659 LUMO: 2.22045 factor:1 | 1 (-1.12078) | -1 | -1 |
| G: -6289.12860 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.26838 HOMO: -6.73482 LUMO: 2.20956 factor:1 | 1 (-0.77408) | -1 | -1 |
| G: -6289.12860 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.37134 HOMO: -6.74026 LUMO: 1.76602 factor:1 | 1 (-0.87705) | -1 | -1 |
| G: -6289.12860 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.18625 HOMO: -6.95523 LUMO: 1.94834 factor:1 | 1 (-0.69196) | -1 | -1 |
| G: -6289.12860 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.00451 HOMO: -6.33209 LUMO: 1.87486 factor:1 | 1 (-0.51021) | -1 | -1 |
| G: -6289.12860 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.50678 HOMO: -6.71033 LUMO: 2.12521 factor:1 | 1 (-1.01248) | -1 | -1 |
| G: -6289.12860 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.17507 HOMO: -6.50080 LUMO: 2.04902 factor:1 | 1 (-0.68077) | -1 | -1 |
| G: -6289.12860 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.76575 HOMO: -6.76475 LUMO: 1.94017 factor:1 | 1 (-1.27145) | -1 | -1 |
| G: -6289.12860 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.65780 HOMO: -6.53073 LUMO: 2.08983 factor:1 | 1 (-1.16350) | -1 | -1 |
| G: -6289.12860 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.14975 HOMO: -6.69944 LUMO: 2.20684 factor:1 | 1 (-1.65546) | -1 | -1 |
| G: -6289.12860 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.18023 HOMO: -6.34570 LUMO: 1.80684 factor:1 | 1 (-1.68594) | -1 | -1 |
| G: -6289.12860 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.04140 HOMO: -6.78380 LUMO: 1.95922 factor:1 | 1 (-1.54710) | -1 | -1 |
| G: -6289.12860 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.36113 HOMO: -6.93618 LUMO: 1.76058 factor:1 | 1 (-1.86684) | -1 | -1 |
| G: -6289.12860 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.41039 HOMO: -6.93346 LUMO: 1.79595 factor:1 | 1 (-0.91610) | -1 | -1 |
| G: -6289.12860 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.26166 HOMO: -6.29671 LUMO: 1.75241 factor:1 | 1 (-0.76736) | -1 | -1 |
| G: -6289.12860 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12553.97194 HOMO: -6.77019 LUMO: 1.74697 factor:1 | 1 (-0.47764) | -1 | -1 |
| G: -6289.12860 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.07330 HOMO: -6.87360 LUMO: 1.91024 factor:1 | 1 (-0.57900) | -1 | -1 |
| G: -6289.12860 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12553.76902 HOMO: -6.32665 LUMO: 1.87759 factor:1 | 1 (-0.27473) | -1 | -1 |
| G: -6289.12860 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12553.41067 HOMO: -6.99877 LUMO: 1.99187 factor:1 | -1 (0.08362) | -1 | -1 |
| G: -6289.12860 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.17548 HOMO: -6.72665 LUMO: 2.12521 factor:1 | 1 (-0.68118) | -1 | -1 |
| G: -6289.12860 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.85171 HOMO: -6.67767 LUMO: 2.43814 factor:1 | 1 (-1.35741) | -1 | -1 |
| G: -6289.12860 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.72523 HOMO: -6.99605 LUMO: 1.79051 factor:1 | 1 (-1.23093) | -1 | -1 |
| G: -6289.12860 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.63233 HOMO: -6.25046 LUMO: 1.77146 factor:1 | 1 (-1.13803) | -1 | -1 |
| G: -6289.12860 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.82349 HOMO: -6.30488 LUMO: 1.90480 factor:1 | 1 (-1.32919) | -1 | -1 |
| G: -6289.12860 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.54321 HOMO: -6.38379 LUMO: 1.68438 factor:1 | 1 (-1.04892) | -1 | -1 |
| G: -6289.12860 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.64433 HOMO: -6.78924 LUMO: 2.01364 factor:1 | 1 (-1.15003) | -1 | -1 |
| G: -6289.12860 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.39890 HOMO: -6.15249 LUMO: 1.98643 factor:1 | 1 (-1.90461) | -1 | -1 |
| G: -6289.12860 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.51724 HOMO: -6.19331 LUMO: 2.14154 factor:1 | 1 (-2.02295) | -1 | -1 |
| G: -6289.12860 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.55733 HOMO: -6.05998 LUMO: 2.12521 factor:1 | 1 (-2.06303) | -1 | -1 |
| G: -6289.12860 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.30592 HOMO: -6.67223 LUMO: 1.91840 factor:1 | 1 (-1.81163) | -1 | -1 |
| G: -6289.12860 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.35501 HOMO: -6.79196 LUMO: 2.18507 factor:1 | 1 (-1.86071) | -1 | -1 |
| G: -6289.12860 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.73402 HOMO: -6.93346 LUMO: 1.78235 factor:1 | 1 (-1.23972) | -1 | -1 |
| G: -6289.12860 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.80036 HOMO: -6.16882 LUMO: 1.80956 factor:1 | 1 (-1.30606) | -1 | -1 |
| G: -6289.12860 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.63363 HOMO: -6.72665 LUMO: 2.07895 factor:1 | 1 (-1.13934) | -1 | -1 |
| G: -6289.12860 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.52204 HOMO: -6.73210 LUMO: 1.97827 factor:1 | 1 (-1.02775) | -1 | -1 |
| G: -6289.12860 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.42841 HOMO: -6.84638 LUMO: 1.87214 factor:1 | 1 (-0.93411) | -1 | -1 |
| G: -6289.12860 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.35205 HOMO: -6.83006 LUMO: 2.36195 factor:1 | 1 (-0.85776) | -1 | -1 |
| G: -6289.12860 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.38996 HOMO: -6.97700 LUMO: 1.91024 factor:1 | 1 (-0.89566) | -1 | -1 |
| G: -6289.12860 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.11594 HOMO: -6.20420 LUMO: 1.81772 factor:1 | 1 (-0.62164) | -1 | -1 |
| G: -6289.12860 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.48307 HOMO: -7.09129 LUMO: 2.10344 factor:1 | 1 (-0.98878) | 1 | 1 |
| G: -6289.12860 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.35400 HOMO: -6.77564 LUMO: 2.14970 factor:1 | 1 (-1.85971) | -1 | -1 |
| G: -6289.12860 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.54952 HOMO: -6.81645 LUMO: 1.85854 factor:1 | 1 (-2.05522) | -1 | -1 |
| G: -6289.12860 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.08924 HOMO: -6.50896 LUMO: 2.04358 factor:1 | 1 (-1.59494) | -1 | -1 |
| G: -6289.12860 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.51860 HOMO: -6.89264 LUMO: 1.66262 factor:1 | 1 (-2.02431) | -1 | -1 |
| G: -6289.12860 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.36355 HOMO: -6.75931 LUMO: 2.23950 factor:1 | 1 (-1.86926) | -1 | -1 |
| G: -6289.12860 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.80575 HOMO: -6.50080 LUMO: 1.67622 factor:1 | 1 (-1.31145) | -1 | -1 |
| G: -6289.12860 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.54626 HOMO: -6.30216 LUMO: 2.24222 factor:1 | 1 (-1.05196) | -1 | -1 |
| G: -6289.12860 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.68245 HOMO: -7.18108 LUMO: 2.10072 factor:1 | 1 (-1.18816) | 1 | 1 |
| G: -6289.12860 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.37311 HOMO: -6.54162 LUMO: 2.35378 factor:1 | 1 (-0.87882) | -1 | -1 |
| G: -6289.12860 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.17839 HOMO: -5.98650 LUMO: 1.48302 factor:1 | 1 (-0.68409) | -1 | -1 |
| G: -6289.12860 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.39826 HOMO: -7.15115 LUMO: 2.14970 factor:1 | 1 (-0.90396) | 1 | 1 |
| G: -6289.12860 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.60539 HOMO: -6.45454 LUMO: 2.15786 factor:1 | 1 (-1.11110) | -1 | -1 |
| G: -6289.12860 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.75625 HOMO: -7.06952 LUMO: 2.14970 factor:1 | 1 (-1.26196) | 1 | 1 |
| G: -6289.12860 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.44792 HOMO: -6.93618 LUMO: 1.86942 factor:1 | 1 (-0.95362) | -1 | -1 |
| G: -6289.12860 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.55932 HOMO: -6.63141 LUMO: 1.92657 factor:1 | 1 (-1.06503) | -1 | -1 |
| G: -6289.12860 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.62261 HOMO: -6.51441 LUMO: -0.44355 factor:1 | 1 (-1.12832) | -1 | -1 |
| G: -6289.12860 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.19605 HOMO: -6.82734 LUMO: -1.03131 factor:1 | 1 (-0.70175) | -1 | -1 |
| G: -6289.12860 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.19891 HOMO: -6.58788 LUMO: -0.82995 factor:1 | 1 (-0.70461) | -1 | -1 |
| G: -6289.12860 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12553.93044 HOMO: -6.43277 LUMO: -0.40817 factor:1 | 1 (-0.43614) | -1 | -1 |
| G: -6289.12860 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.33929 HOMO: -6.78924 LUMO: -0.72110 factor:1 | 1 (-0.84500) | -1 | -1 |
| G: -6289.12860 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.55102 HOMO: -7.28177 LUMO: 0.36735 factor:1 | 1 (-1.05673) | -1 | -1 |
| G: -6289.12860 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.54346 HOMO: -6.47903 LUMO: -0.46259 factor:1 | 1 (-1.04916) | -1 | -1 |
| G: -6289.12860 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.52451 HOMO: -6.67495 LUMO: -0.75376 factor:1 | 1 (-2.03021) | -1 | -1 |
| G: -6289.12860 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.58799 HOMO: -6.71033 LUMO: -0.71838 factor:1 | 1 (-2.09370) | -1 | -1 |
| G: -6289.12860 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.34230 HOMO: -6.79740 LUMO: -0.79185 factor:1 | 1 (-1.84801) | -1 | -1 |
| G: -6289.12860 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.37732 HOMO: -6.08719 LUMO: -0.63675 factor:1 | 1 (-1.88303) | -1 | -1 |
| G: -6289.12860 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.20799 HOMO: -6.84094 LUMO: 0.42994 factor:1 | 1 (-1.71369) | -1 | -1 |
| G: -6289.12860 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.24102 HOMO: -6.59604 LUMO: 0.25851 factor:1 | 1 (-1.74673) | -1 | -1 |
| G: -6289.12860 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.19558 HOMO: -6.82462 LUMO: 0.08708 factor:1 | 1 (-1.70128) | -1 | -1 |
| G: -6289.12860 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.38140 HOMO: -6.54706 LUMO: 0.44082 factor:1 | 1 (-1.88711) | -1 | -1 |
| G: -6289.12860 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.28284 HOMO: -6.99333 LUMO: 0.32109 factor:1 | 1 (-1.78855) | -1 | -1 |
| G: -6289.12860 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.01748 HOMO: -6.29944 LUMO: -0.57144 factor:1 | 1 (-1.52318) | -1 | -1 |
| G: -6289.12860 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.35865 HOMO: -6.57699 LUMO: -0.46531 factor:1 | 1 (-1.86436) | -1 | -1 |
| G: -6289.12860 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.25729 HOMO: -6.24773 LUMO: -0.53879 factor:1 | 1 (-1.76300) | -1 | -1 |
| G: -6289.12860 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.27884 HOMO: -6.96067 LUMO: -0.67212 factor:1 | 1 (-1.78455) | -1 | -1 |
| G: -6289.12860 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.10858 HOMO: -7.24095 LUMO: -0.09252 factor:1 | 1 (-1.61429) | -1 | -1 |
| G: -6289.12860 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.32355 HOMO: -6.33481 LUMO: -0.46531 factor:1 | 1 (-1.82926) | -1 | -1 |
| G: -6289.12860 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.35972 HOMO: -6.43549 LUMO: -0.33198 factor:1 | 1 (-1.86542) | -1 | -1 |
| G: -6289.12860 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.51466 HOMO: -6.53073 LUMO: 0.44899 factor:1 | 1 (-2.02036) | -1 | -1 |
| G: -6289.12860 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.34935 HOMO: -6.69128 LUMO: 0.47620 factor:1 | 1 (-1.85505) | -1 | -1 |
| G: -6289.12860 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.16924 HOMO: -6.65318 LUMO: 0.52246 factor:1 | 1 (-1.67494) | -1 | -1 |
| G: -6289.12860 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.10091 HOMO: -6.71305 LUMO: 0.41089 factor:1 | 1 (-1.60661) | -1 | -1 |
| G: -6289.12860 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.39294 HOMO: -6.70216 LUMO: 0.19864 factor:1 | 1 (-1.89865) | -1 | -1 |
| G: -6289.12860 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.40271 HOMO: -6.41100 LUMO: 0.34558 factor:1 | 1 (-1.90842) | -1 | -1 |
| G: -6289.12860 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.43825 HOMO: -7.01237 LUMO: 0.02993 factor:1 | 1 (-1.94395) | -1 | -1 |
| G: -6289.12860 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.23220 HOMO: -6.85999 LUMO: 0.18776 factor:1 | 1 (-1.73791) | -1 | -1 |
| G: -6289.12860 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.40211 HOMO: -6.62869 LUMO: 0.48708 factor:1 | 1 (-1.90782) | -1 | -1 |
| G: -6289.12860 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.02986 HOMO: -6.43821 LUMO: -0.45715 factor:1 | 1 (-1.53557) | -1 | -1 |
| G: -6289.12860 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.99214 HOMO: -6.43277 LUMO: -0.72110 factor:1 | 1 (-1.49785) | -1 | -1 |
| G: -6289.12860 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.32070 HOMO: -7.10761 LUMO: 0.43266 factor:1 | 1 (-1.82640) | -1 | -1 |
| G: -6289.12860 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.17234 HOMO: -6.57699 LUMO: -0.61498 factor:1 | 1 (-1.67804) | -1 | -1 |
| G: -6289.12860 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.45336 HOMO: -6.82189 LUMO: -0.75648 factor:1 | 1 (-0.95907) | -1 | -1 |
| G: -6289.12860 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.56604 HOMO: -6.55794 LUMO: -0.67212 factor:1 | 1 (-1.07175) | -1 | -1 |
| G: -6289.12860 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.59407 HOMO: -6.69128 LUMO: 1.88575 factor:1 | 1 (-1.09978) | -1 | -1 |
| G: -6289.12860 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.70833 HOMO: -6.65591 LUMO: 1.70888 factor:1 | 1 (-1.21404) | -1 | -1 |
| G: -6289.12860 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.32947 HOMO: -6.58788 LUMO: 1.68438 factor:1 | 1 (-0.83517) | -1 | -1 |
| G: -6289.12860 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.38666 HOMO: -6.46270 LUMO: 1.72520 factor:1 | 1 (-0.89237) | -1 | -1 |
| G: -6289.12860 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.43706 HOMO: -6.57427 LUMO: 1.73881 factor:1 | 1 (-0.94277) | -1 | -1 |
| G: -6289.12860 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.62566 HOMO: -6.45182 LUMO: 1.75241 factor:1 | 1 (-1.13137) | -1 | -1 |
| G: -6289.12860 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.51948 HOMO: -6.51441 LUMO: 1.78779 factor:1 | 1 (-1.02519) | -1 | -1 |
| G: -6289.12860 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.48922 HOMO: -6.67495 LUMO: 2.11705 factor:1 | 1 (-0.99493) | -1 | -1 |
| G: -6289.12860 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.33834 HOMO: -6.22597 LUMO: 1.96466 factor:1 | 1 (-0.84404) | -1 | -1 |
| G: -6289.12860 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.45330 HOMO: -6.68040 LUMO: 2.30753 factor:1 | 1 (-1.95900) | -1 | -1 |
| G: -6289.12860 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.46927 HOMO: -6.65046 LUMO: 2.18235 factor:1 | 1 (-1.97498) | -1 | -1 |
| G: -6289.12860 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.21560 HOMO: -6.38651 LUMO: 1.76874 factor:1 | 1 (-1.72131) | -1 | -1 |
| G: -6289.12860 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.54524 HOMO: -6.41644 LUMO: 2.09256 factor:1 | 1 (-2.05095) | -1 | -1 |
| G: -6289.12860 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.30859 HOMO: -6.14977 LUMO: 2.28031 factor:1 | 1 (-1.81429) | -1 | -1 |
| G: -6289.12860 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.15718 HOMO: -6.70489 LUMO: 2.43814 factor:1 | 1 (-1.66289) | -1 | -1 |
| G: -6289.12860 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.97383 HOMO: -6.78924 LUMO: 2.27215 factor:1 | 1 (-1.47954) | -1 | -1 |
| G: -6289.12860 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.38042 HOMO: -6.86271 LUMO: 2.31025 factor:1 | 1 (-1.88613) | -1 | -1 |
| G: -6289.12860 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.17073 HOMO: -6.51168 LUMO: 2.04630 factor:1 | 1 (-1.67644) | -1 | -1 |
| G: -6289.12860 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.34355 HOMO: -6.72665 LUMO: 2.13337 factor:1 | 1 (-1.84926) | -1 | -1 |
| G: -6289.12860 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.29865 HOMO: -6.45998 LUMO: 2.16058 factor:1 | 1 (-1.80436) | -1 | -1 |
| G: -6289.12860 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.10551 HOMO: -6.83822 LUMO: 2.20684 factor:1 | 1 (-1.61121) | -1 | -1 |
| G: -6289.12860 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.00766 HOMO: -6.68856 LUMO: 2.19324 factor:1 | 1 (-1.51336) | -1 | -1 |
| G: -6289.12860 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.39501 HOMO: -6.71577 LUMO: 2.16058 factor:1 | 1 (-1.90072) | -1 | -1 |
| G: -6289.12860 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.25174 HOMO: -6.82462 LUMO: 1.90208 factor:1 | 1 (-1.75745) | -1 | -1 |
| G: -6289.12860 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.95043 HOMO: -6.61509 LUMO: 2.23950 factor:1 | 1 (-1.45614) | -1 | -1 |
| G: -6289.12860 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.90599 HOMO: -6.73754 LUMO: 1.84221 factor:1 | 1 (-1.41170) | -1 | -1 |
| G: -6289.12860 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.79331 HOMO: -6.56611 LUMO: 1.94561 factor:1 | 1 (-1.29902) | -1 | -1 |
| G: -6289.12860 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.46476 HOMO: -6.67767 LUMO: 1.51840 factor:1 | 1 (-0.97047) | -1 | -1 |
| G: -6289.12860 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.19547 HOMO: -6.35658 LUMO: 2.16603 factor:1 | 1 (-1.70117) | -1 | -1 |
| G: -6289.12860 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.06020 HOMO: -6.35114 LUMO: 2.08983 factor:1 | 1 (-1.56591) | -1 | -1 |
| G: -6289.12860 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.85639 HOMO: -6.35114 LUMO: 2.10616 factor:1 | 1 (-1.36209) | -1 | -1 |
| G: -6289.12860 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.24048 HOMO: -6.71305 LUMO: 2.01636 factor:1 | 1 (-1.74618) | -1 | -1 |
| G: -6289.12860 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.06317 HOMO: -6.24773 LUMO: 1.98915 factor:1 | 1 (-1.56887) | -1 | -1 |
| G: -6289.12860 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.20154 HOMO: -6.53617 LUMO: 2.42726 factor:1 | 1 (-1.70724) | -1 | -1 |
| G: -6289.12860 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.41819 HOMO: -6.59332 LUMO: 1.82316 factor:1 | 1 (-1.92390) | -1 | -1 |
| G: -6289.12860 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.97078 HOMO: -6.41372 LUMO: 1.77418 factor:1 | 1 (-1.47649) | -1 | -1 |
| G: -6289.12860 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.90708 HOMO: -6.40284 LUMO: 1.88575 factor:1 | 1 (-1.41279) | -1 | -1 |
| G: -6289.12860 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.99133 HOMO: -6.11168 LUMO: 1.70888 factor:1 | 1 (-1.49703) | -1 | -1 |
| G: -6289.12860 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.35686 HOMO: -6.44910 LUMO: 2.23405 factor:1 | 1 (-1.86256) | -1 | -1 |
| G: -6289.12860 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.15615 HOMO: -6.24773 LUMO: 2.12793 factor:1 | 1 (-1.66185) | -1 | -1 |
| G: -6289.12860 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.22790 HOMO: -6.07358 LUMO: 1.89663 factor:1 | 1 (-1.73361) | -1 | -1 |
| G: -6289.12860 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.13960 HOMO: -6.66679 LUMO: 1.96738 factor:1 | 1 (-1.64531) | -1 | -1 |
| G: -6289.12860 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.36355 HOMO: -6.68312 LUMO: 1.78235 factor:1 | 1 (-1.86926) | -1 | -1 |
| G: -6289.12860 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.86058 HOMO: -6.70761 LUMO: 1.97555 factor:1 | 1 (-1.36628) | -1 | -1 |
| G: -6289.12860 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.73361 HOMO: -6.15794 LUMO: 2.00548 factor:1 | 1 (-1.23932) | -1 | -1 |
| G: -6289.12860 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.83489 HOMO: -6.52257 LUMO: 1.96738 factor:1 | 1 (-1.34060) | -1 | -1 |
| G: -6289.12860 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.46999 HOMO: -6.25590 LUMO: 1.86670 factor:1 | 1 (-0.97569) | -1 | -1 |
| G: -6289.12860 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.11628 HOMO: -6.30216 LUMO: 1.84765 factor:1 | 1 (-1.62199) | -1 | -1 |
| G: -6289.12860 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.91271 HOMO: -6.76747 LUMO: 2.20956 factor:1 | 1 (-1.41842) | -1 | -1 |
| G: -6289.12860 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.90833 HOMO: -6.14161 LUMO: 1.80684 factor:1 | 1 (-1.41404) | -1 | -1 |
| G: -6289.12860 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.82675 HOMO: -6.81373 LUMO: 1.91024 factor:1 | 1 (-1.33246) | -1 | -1 |
| G: -6289.12860 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.64019 HOMO: -6.81917 LUMO: 2.34834 factor:1 | 1 (-1.14590) | -1 | -1 |
| G: -6289.12860 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.11182 HOMO: -6.72121 LUMO: 1.90208 factor:1 | 1 (-1.61753) | -1 | -1 |
| G: -6289.12860 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.80557 HOMO: -7.51851 LUMO: 0.26939 factor:1 | 1 (-2.31128) | -1 | -1 |
| G: -6289.12860 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12556.58268 HOMO: -6.65318 LUMO: -0.57144 factor:1 | 1 (-3.08838) | -1 | -1 |
| G: -6289.12860 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.45983 HOMO: -6.77564 LUMO: -0.72654 factor:1 | 1 (-1.96553) | -1 | -1 |
| G: -6289.12860 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.60160 HOMO: -6.80557 LUMO: -0.60954 factor:1 | 1 (-2.10730) | -1 | -1 |
| G: -6289.12860 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.80664 HOMO: -7.35524 LUMO: 0.27483 factor:1 | 1 (-2.31234) | -1 | -1 |
| G: -6289.12860 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.39713 HOMO: -6.94979 LUMO: -0.83811 factor:1 | 1 (-1.90284) | -1 | -1 |
| G: -6289.12860 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.89643 HOMO: -6.13345 LUMO: -0.67212 factor:1 | 1 (-2.40214) | -1 | -1 |
| G: -6289.12860 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12556.40423 HOMO: -6.47359 LUMO: -0.59321 factor:1 | 1 (-2.90993) | -1 | -1 |
| G: -6289.12860 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12556.12193 HOMO: -6.52257 LUMO: -0.54695 factor:1 | 1 (-2.62764) | -1 | -1 |
| G: -6289.12860 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12556.58015 HOMO: -6.61781 LUMO: -0.69661 factor:1 | 1 (-3.08585) | -1 | -1 |
| G: -6289.12860 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.42173 HOMO: -6.77564 LUMO: -0.80001 factor:1 | 1 (-1.92744) | -1 | -1 |
| G: -6289.12860 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.23816 HOMO: -7.35252 LUMO: -1.00410 factor:1 | 1 (-1.74387) | -1 | -1 |
| G: -6289.12860 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.05566 HOMO: -6.35386 LUMO: -0.38912 factor:1 | 1 (-1.56136) | -1 | -1 |
| G: -6289.12860 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12556.52153 HOMO: -6.80285 LUMO: -0.52246 factor:1 | 1 (-3.02724) | -1 | -1 |
| G: -6289.12860 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.73961 HOMO: -7.23279 LUMO: 0.30477 factor:1 | 1 (-2.24532) | -1 | -1 |
| G: -6289.12860 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12556.66714 HOMO: -7.13483 LUMO: -0.76192 factor:1 | 1 (-3.17285) | -1 | -1 |
| G: -6289.12860 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.36274 HOMO: -6.71849 LUMO: -0.48164 factor:1 | 1 (-1.86844) | -1 | -1 |
| G: -6289.12860 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12556.13257 HOMO: -6.85455 LUMO: -0.69389 factor:1 | 1 (-2.63828) | -1 | -1 |
| G: -6289.12860 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.88773 HOMO: -6.96339 LUMO: -0.73743 factor:1 | 1 (-2.39343) | -1 | -1 |
| G: -6289.12860 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.67365 HOMO: -7.50490 LUMO: 0.28844 factor:1 | 1 (-2.17936) | -1 | -1 |
| G: -6289.12860 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.52623 HOMO: -6.63958 LUMO: -0.50069 factor:1 | 1 (-1.03194) | -1 | -1 |
| G: -6289.12860 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.39515 HOMO: -6.78924 LUMO: -0.69661 factor:1 | 1 (-0.90086) | -1 | -1 |
| G: -6289.12860 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.93986 HOMO: -7.44776 LUMO: 0.33742 factor:1 | 1 (-2.44557) | -1 | -1 |
| G: -6289.12860 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.39808 HOMO: -6.15249 LUMO: 0.66396 factor:1 | 1 (-1.90379) | -1 | -1 |
| G: -6289.12860 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.79034 HOMO: -6.17426 LUMO: 0.55511 factor:1 | 1 (-2.29604) | -1 | -1 |
| G: -6289.12860 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.34219 HOMO: -6.83550 LUMO: 0.28844 factor:1 | 1 (-1.84790) | -1 | -1 |
| G: -6289.12860 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.28611 HOMO: -6.32393 LUMO: 0.47620 factor:1 | 1 (-1.79182) | -1 | -1 |
| G: -6289.12860 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.39599 HOMO: -6.32937 LUMO: 0.45987 factor:1 | 1 (-1.90169) | -1 | -1 |
| G: -6289.12860 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.31789 HOMO: -7.37429 LUMO: 0.09252 factor:1 | 1 (-1.82360) | -1 | -1 |
| G: -6289.12860 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.45928 HOMO: -6.54434 LUMO: -0.39729 factor:1 | 1 (-1.96499) | -1 | -1 |
| G: -6289.12860 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.24505 HOMO: -7.35524 LUMO: 0.28028 factor:1 | 1 (-1.75075) | -1 | -1 |
| G: -6289.12860 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.11258 HOMO: -6.95523 LUMO: -0.86804 factor:1 | 1 (-1.61829) | -1 | -1 |
| G: -6289.12860 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.18151 HOMO: -6.63958 LUMO: -0.65307 factor:1 | 1 (-1.68721) | -1 | -1 |
| G: -6289.12860 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.89111 HOMO: -6.73482 LUMO: -0.67212 factor:1 | 1 (-1.39681) | -1 | -1 |
| G: -6289.12860 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.63368 HOMO: -6.37835 LUMO: -0.53606 factor:1 | 1 (-2.13939) | -1 | -1 |
| G: -6289.12860 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.82449 HOMO: -6.71849 LUMO: -0.61226 factor:1 | 1 (-2.33019) | -1 | -1 |
| G: -6289.12860 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.62680 HOMO: -6.68584 LUMO: -1.11022 factor:1 | 1 (-2.13250) | -1 | -1 |
| G: -6289.12860 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.85341 HOMO: -6.80285 LUMO: -0.79185 factor:1 | 1 (-2.35912) | -1 | -1 |
| G: -6289.12860 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12556.43340 HOMO: -7.14571 LUMO: -0.94696 factor:1 | 1 (-2.93910) | -1 | -1 |
| G: -6289.12860 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.65975 HOMO: -7.16204 LUMO: -0.66124 factor:1 | 1 (-2.16545) | -1 | -1 |
| G: -6289.12860 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12556.13021 HOMO: -6.54978 LUMO: -0.54967 factor:1 | 1 (-2.63591) | -1 | -1 |
| G: -6289.12860 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12556.21704 HOMO: -6.75114 LUMO: -0.70750 factor:1 | 1 (-2.72274) | -1 | -1 |
| G: -6289.12860 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.49700 HOMO: -7.22190 LUMO: 0.39184 factor:1 | 1 (-2.00270) | -1 | -1 |
| G: -6289.12860 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12556.06212 HOMO: -7.43959 LUMO: 0.30477 factor:1 | 1 (-2.56783) | -1 | -1 |
| G: -6289.12860 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.34369 HOMO: -6.87360 LUMO: -0.77552 factor:1 | 1 (-1.84939) | -1 | -1 |
| G: -6289.12860 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.41808 HOMO: -6.82734 LUMO: -0.59593 factor:1 | 1 (-1.92379) | -1 | -1 |
| G: -6289.12860 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.62152 HOMO: -6.65318 LUMO: -0.46259 factor:1 | 1 (-2.12722) | -1 | -1 |
| G: -6289.12860 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.46562 HOMO: -7.05863 LUMO: -1.17009 factor:1 | 1 (-1.97133) | -1 | -1 |
| G: -6289.12860 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.23713 HOMO: -6.57427 LUMO: -0.48708 factor:1 | 1 (-1.74283) | -1 | -1 |
| G: -6289.12860 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.25264 HOMO: -6.60420 LUMO: -0.38096 factor:1 | 1 (-1.75835) | -1 | -1 |
| G: -6289.12860 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.60455 HOMO: -6.72121 LUMO: -0.66668 factor:1 | 1 (-1.11025) | -1 | -1 |
| G: -6289.12860 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.38381 HOMO: -6.52257 LUMO: -0.19320 factor:1 | 1 (-0.88951) | -1 | -1 |
| G: -6289.12860 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.30209 HOMO: -6.28039 LUMO: -0.27211 factor:1 | 1 (-0.80780) | -1 | -1 |
| G: -6289.12860 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.56188 HOMO: -6.71849 LUMO: -0.42722 factor:1 | 1 (-1.06758) | -1 | -1 |
| G: -6289.12860 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.51208 HOMO: -6.27495 LUMO: 0.27756 factor:1 | 1 (-1.01779) | -1 | -1 |
| G: -6289.12860 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.11390 HOMO: -6.21780 LUMO: 0.46531 factor:1 | 1 (-0.61960) | -1 | -1 |
| G: -6289.12860 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.38879 HOMO: -6.52257 LUMO: -0.64491 factor:1 | 1 (-0.89449) | -1 | -1 |
| G: -6289.12860 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.31853 HOMO: -6.73754 LUMO: 1.83133 factor:1 | 1 (-0.82423) | -1 | -1 |
| G: -6289.12860 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.34990 HOMO: -6.67223 LUMO: 1.88847 factor:1 | 1 (-0.85561) | -1 | -1 |
| G: -6289.12860 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.18759 HOMO: -6.82189 LUMO: 1.59187 factor:1 | 1 (-0.69329) | -1 | -1 |
| G: -6289.12860 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.54659 HOMO: -6.43277 LUMO: 1.76330 factor:1 | 1 (-1.05229) | -1 | -1 |
| G: -6289.12860 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.32462 HOMO: -6.48175 LUMO: 1.77962 factor:1 | 1 (-0.83033) | -1 | -1 |
| G: -6289.12860 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.71787 HOMO: -6.50352 LUMO: 1.68438 factor:1 | 1 (-2.22358) | -1 | -1 |
| G: -6289.12860 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12556.50834 HOMO: -6.31576 LUMO: 2.03813 factor:1 | 1 (-3.01404) | -1 | -1 |
| G: -6289.12860 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12556.25900 HOMO: -6.27495 LUMO: 1.99459 factor:1 | 1 (-2.76470) | -1 | -1 |
| G: -6289.12860 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.60573 HOMO: -6.23957 LUMO: 2.17147 factor:1 | 1 (-2.11144) | -1 | -1 |
| G: -6289.12860 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.16707 HOMO: -6.78108 LUMO: 2.16875 factor:1 | 1 (-0.67277) | -1 | -1 |
| G: -6289.12860 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.39722 HOMO: -6.34297 LUMO: 2.10344 factor:1 | 1 (-0.90293) | -1 | -1 |
| G: -6289.12860 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.86778 HOMO: -6.30216 LUMO: 2.00004 factor:1 | 1 (-2.37349) | -1 | -1 |
| G: -6289.12860 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.19786 HOMO: -6.72665 LUMO: 2.09528 factor:1 | 1 (-1.70357) | -1 | -1 |
| G: -6289.12860 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12556.00384 HOMO: -6.86543 LUMO: 1.91568 factor:1 | 1 (-2.50954) | -1 | -1 |
| G: -6289.12860 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.90718 HOMO: -5.83956 LUMO: 1.89391 factor:1 | 1 (-2.41289) | -1 | -1 |
| G: -6289.12860 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.69028 HOMO: -6.42189 LUMO: 2.03269 factor:1 | 1 (-2.19599) | -1 | -1 |
| G: -6289.12860 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.97155 HOMO: -6.07630 LUMO: 1.80956 factor:1 | 1 (-1.47725) | -1 | -1 |
| G: -6289.12860 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.27920 HOMO: -6.43277 LUMO: 1.81772 factor:1 | 1 (-1.78490) | -1 | -1 |
| G: -6289.12860 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.40753 HOMO: -7.03959 LUMO: 1.78779 factor:1 | 1 (-1.91323) | -1 | -1 |
| G: -6289.12860 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.37204 HOMO: -6.72121 LUMO: 2.29664 factor:1 | 1 (-1.87775) | -1 | -1 |
| G: -6289.12860 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.35400 HOMO: -6.62869 LUMO: 2.04630 factor:1 | 1 (-1.85971) | -1 | -1 |
| G: -6289.12860 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.26965 HOMO: -6.63958 LUMO: 1.84221 factor:1 | 1 (-1.77535) | -1 | -1 |
| G: -6289.12860 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.56494 HOMO: -6.70761 LUMO: 1.67350 factor:1 | 1 (-2.07065) | -1 | -1 |
| G: -6289.12860 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.58816 HOMO: -6.00283 LUMO: 1.64357 factor:1 | 1 (-2.09386) | -1 | -1 |
| G: -6289.12860 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.36513 HOMO: -6.48719 LUMO: 1.70343 factor:1 | 1 (-1.87084) | -1 | -1 |
| G: -6289.12860 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.40862 HOMO: -6.13345 LUMO: 1.44492 factor:1 | 1 (-1.91432) | -1 | -1 |
| G: -6289.12860 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.10551 HOMO: -6.11168 LUMO: 1.70071 factor:1 | 1 (-1.61121) | -1 | -1 |
| G: -6289.12860 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.22761 HOMO: -6.09535 LUMO: 1.82316 factor:1 | 1 (-0.73332) | -1 | -1 |
| G: -6289.12860 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.08201 HOMO: -6.81101 LUMO: 1.63540 factor:1 | 1 (-0.58771) | -1 | -1 |
| G: -6289.12860 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.09991 HOMO: -6.80013 LUMO: 2.12249 factor:1 | 1 (-0.60562) | -1 | -1 |
| G: -6289.12860 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12553.83993 HOMO: -6.48447 LUMO: 1.94561 factor:1 | 1 (-0.34564) | -1 | -1 |
| G: -6289.12860 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.28459 HOMO: -6.72393 LUMO: 2.06534 factor:1 | 1 (-0.79030) | -1 | -1 |
| G: -6289.12860 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.99962 HOMO: -6.34570 LUMO: 1.98915 factor:1 | 1 (-2.50533) | -1 | -1 |
| G: -6289.12860 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.73978 HOMO: -6.31304 LUMO: 1.87759 factor:1 | 1 (-2.24548) | -1 | -1 |
| G: -6289.12860 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12556.05709 HOMO: -6.77564 LUMO: 1.81228 factor:1 | 1 (-2.56280) | -1 | -1 |
| G: -6289.12860 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.32848 HOMO: -6.58516 LUMO: 2.34834 factor:1 | 1 (-1.83418) | -1 | -1 |
| G: -6289.12860 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.05522 HOMO: -6.68040 LUMO: 2.20412 factor:1 | 1 (-1.56093) | -1 | -1 |
| G: -6289.12860 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.89976 HOMO: -6.20964 LUMO: 2.17147 factor:1 | 1 (-1.40547) | -1 | -1 |
| G: -6289.12860 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.09280 HOMO: -6.54706 LUMO: 2.03813 factor:1 | 1 (-1.59851) | -1 | -1 |
| G: -6289.12860 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.24516 HOMO: -6.54162 LUMO: 2.17419 factor:1 | 1 (-1.75086) | -1 | -1 |
| G: -6289.12860 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.22695 HOMO: -6.75659 LUMO: 2.22589 factor:1 | 1 (-1.73266) | -1 | -1 |
| G: -6289.12860 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.92885 HOMO: -6.59604 LUMO: 2.59325 factor:1 | 1 (-1.43456) | -1 | -1 |
| G: -6289.12860 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.04507 HOMO: -6.11712 LUMO: 2.02181 factor:1 | 1 (-1.55078) | -1 | -1 |
| G: -6289.12860 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.79405 HOMO: -6.63141 LUMO: 2.09256 factor:1 | 1 (-1.29975) | -1 | -1 |
| G: -6289.12860 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.23476 HOMO: -6.61781 LUMO: 1.86126 factor:1 | 1 (-1.74047) | -1 | -1 |
| G: -6289.12860 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.38944 HOMO: -6.63958 LUMO: 1.77146 factor:1 | 1 (-0.89515) | -1 | -1 |
| G: -6289.12860 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.58509 HOMO: -6.60420 LUMO: 1.54561 factor:1 | 1 (-1.09080) | -1 | -1 |
| G: -6289.12860 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.52014 HOMO: -6.52529 LUMO: 2.05174 factor:1 | 1 (-1.02584) | -1 | -1 |
| G: -6289.12860 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.48637 HOMO: -6.80285 LUMO: 2.13609 factor:1 | 1 (-0.99207) | -1 | -1 |
| G: -6289.12860 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.19240 HOMO: -6.51168 LUMO: 2.25855 factor:1 | 1 (-0.69811) | -1 | -1 |
| G: -6289.12860 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.33186 HOMO: -6.64774 LUMO: 2.46263 factor:1 | 1 (-0.83757) | -1 | -1 |
| G: -6289.12860 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.55497 HOMO: -6.40828 LUMO: 1.99732 factor:1 | 1 (-1.06067) | -1 | -1 |
| G: -6289.12860 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.78414 HOMO: -5.97562 LUMO: 1.56465 factor:1 | 1 (-1.28985) | -1 | -1 |
| G: -6289.12860 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.75535 HOMO: -6.75659 LUMO: 2.23405 factor:1 | 1 (-1.26106) | -1 | -1 |
| G: -6289.12860 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.48022 HOMO: -6.68584 LUMO: 2.09528 factor:1 | 1 (-0.98592) | -1 | -1 |
| G: -6289.12860 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.55739 HOMO: -6.86543 LUMO: 1.95106 factor:1 | 1 (-1.06309) | -1 | -1 |
| G: -6289.12860 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.23123 HOMO: -6.47359 LUMO: 1.82316 factor:1 | 1 (-0.73694) | -1 | -1 |
| G: -6289.12860 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.33513 HOMO: -6.87632 LUMO: 2.08439 factor:1 | 1 (-0.84083) | -1 | -1 |
| G: -6289.12860 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.20522 HOMO: -6.33753 LUMO: 2.16603 factor:1 | 1 (-0.71092) | -1 | -1 |
| G: -6289.12860 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.04503 HOMO: -6.92258 LUMO: 1.72248 factor:1 | 1 (-0.55073) | -1 | -1 |
| G: -6289.12860 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.33567 HOMO: -6.62597 LUMO: 2.10344 factor:1 | 1 (-0.84138) | -1 | -1 |
| G: -6289.12860 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.57415 HOMO: -6.63141 LUMO: 1.94017 factor:1 | 1 (-1.07986) | -1 | -1 |
| G: -6289.12860 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.62776 HOMO: -6.48447 LUMO: 1.91840 factor:1 | 1 (-1.13346) | -1 | -1 |
| G: -6289.12860 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.35330 HOMO: -6.41372 LUMO: 1.61364 factor:1 | 1 (-0.85901) | -1 | -1 |
| G: -6289.12860 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.57284 HOMO: -6.37291 LUMO: 1.79051 factor:1 | 1 (-1.07855) | -1 | -1 |
| G: -6289.12860 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.47042 HOMO: -6.13073 LUMO: 1.77962 factor:1 | 1 (-0.97613) | -1 | -1 |
| G: -6289.12860 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.67026 HOMO: -6.13073 LUMO: 1.98915 factor:1 | 1 (-1.17597) | -1 | -1 |
| G: -6289.12860 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.17052 HOMO: -6.44094 LUMO: 1.58370 factor:1 | 1 (-1.67622) | -1 | -1 |
| G: -6289.12860 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.33591 HOMO: -6.87087 LUMO: -0.82995 factor:1 | 1 (-1.84161) | -1 | -1 |
| G: -6289.12860 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.04330 HOMO: -6.67223 LUMO: 1.08029 factor:1 | 1 (-1.54901) | -1 | -1 |
| G: -6289.12860 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.11054 HOMO: -6.82462 LUMO: 0.91702 factor:1 | 1 (-1.61625) | -1 | -1 |
| G: -6289.12860 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.02442 HOMO: -6.65863 LUMO: 1.52656 factor:1 | 1 (-1.53012) | -1 | -1 |
| G: -6289.12860 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.08181 HOMO: -6.78924 LUMO: 0.86260 factor:1 | 1 (-1.58751) | -1 | -1 |
| G: -6289.12860 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.56985 HOMO: -6.68584 LUMO: 0.94424 factor:1 | 1 (-1.07556) | -1 | -1 |
| G: -6289.12860 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.31379 HOMO: -6.58788 LUMO: 1.00138 factor:1 | 1 (-0.81950) | -1 | -1 |
| G: -6289.12860 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.13295 HOMO: -6.79740 LUMO: 0.91430 factor:1 | 1 (-0.63865) | -1 | -1 |
| G: -6289.12860 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12553.95498 HOMO: -6.67223 LUMO: 0.80274 factor:1 | 1 (-0.46069) | -1 | -1 |
| G: -6289.12860 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.25401 HOMO: -6.95251 LUMO: 0.90614 factor:1 | 1 (-0.75971) | -1 | -1 |
| G: -6289.12860 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.38432 HOMO: -7.19469 LUMO: 1.34152 factor:1 | 1 (-0.89003) | -1 | -1 |
| G: -6289.12860 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.34198 HOMO: -6.59332 LUMO: -0.76464 factor:1 | 1 (-0.84769) | -1 | -1 |
| G: -6289.12860 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.29774 HOMO: -6.77564 LUMO: -0.90886 factor:1 | 1 (-0.80344) | -1 | -1 |
| G: -6289.12860 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.05771 HOMO: -6.57971 LUMO: -0.41633 factor:1 | 1 (-0.56341) | -1 | -1 |
| G: -6289.12860 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.25414 HOMO: -6.68856 LUMO: -0.58232 factor:1 | 1 (-0.75985) | -1 | -1 |
| G: -6289.12860 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.15757 HOMO: -6.87087 LUMO: -0.71022 factor:1 | 1 (-0.66328) | -1 | -1 |
| G: -6289.12860 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12553.84864 HOMO: -6.67767 LUMO: -0.74559 factor:1 | 1 (-0.35435) | -1 | -1 |
| G: -6289.12860 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.50375 HOMO: -6.68040 LUMO: -0.65307 factor:1 | 1 (-1.00946) | -1 | -1 |
| G: -6289.12860 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.16968 HOMO: -6.32937 LUMO: 0.80274 factor:1 | 1 (-0.67539) | -1 | -1 |
| G: -6289.12860 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.49959 HOMO: -6.29671 LUMO: 0.82723 factor:1 | 1 (-1.00530) | -1 | -1 |
| G: -6289.12860 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.33608 HOMO: -6.67767 LUMO: 0.59321 factor:1 | 1 (-0.84178) | -1 | -1 |
| G: -6289.12860 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.13009 HOMO: -6.77836 LUMO: 0.50341 factor:1 | 1 (-0.63579) | -1 | -1 |
| G: -6289.12860 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12553.82959 HOMO: -6.61781 LUMO: 0.42450 factor:1 | 1 (-0.33530) | -1 | -1 |
| G: -6289.12860 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.32528 HOMO: -6.83278 LUMO: 0.39457 factor:1 | 1 (-0.83098) | -1 | -1 |
| G: -6289.12860 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.51233 HOMO: -6.56883 LUMO: 0.64219 factor:1 | 1 (-1.01803) | -1 | -1 |
| G: -6289.12860 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.45235 HOMO: -6.71577 LUMO: 0.40001 factor:1 | 1 (-0.95806) | -1 | -1 |
| G: -6289.12860 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.26253 HOMO: -6.86543 LUMO: -0.74287 factor:1 | 1 (-0.76823) | -1 | -1 |
| G: -6289.12860 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.26508 HOMO: -6.68584 LUMO: -0.69389 factor:1 | 1 (-0.77079) | -1 | -1 |
| G: -6289.12860 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12553.90959 HOMO: -6.61237 LUMO: -0.48980 factor:1 | 1 (-0.41530) | -1 | -1 |
| G: -6289.12860 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.08103 HOMO: -6.80285 LUMO: -0.58232 factor:1 | 1 (-0.58673) | -1 | -1 |
| G: -6289.12860 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.10432 HOMO: -6.88992 LUMO: -0.70205 factor:1 | 1 (-0.61002) | -1 | -1 |
| G: -6289.12860 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12553.83237 HOMO: -6.95251 LUMO: -0.71838 factor:1 | 1 (-0.33807) | -1 | -1 |
| G: -6289.12860 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.36974 HOMO: -7.52123 LUMO: 0.27211 factor:1 | 1 (-0.87544) | -1 | -1 |
| G: -6289.12860 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.66830 HOMO: -6.76747 LUMO: -0.74015 factor:1 | 1 (-1.17401) | -1 | -1 |
| G: -6289.12860 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.43494 HOMO: -6.55250 LUMO: -0.49797 factor:1 | 1 (-0.94064) | -1 | -1 |
| G: -6289.12860 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.58071 HOMO: -6.50896 LUMO: -0.46804 factor:1 | 1 (-1.08641) | -1 | -1 |
| G: -6289.12860 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.66626 HOMO: -7.45320 LUMO: 0.08436 factor:1 | 1 (-1.17197) | -1 | -1 |
| G: -6289.12860 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.72863 HOMO: -6.82462 LUMO: -0.70477 factor:1 | 1 (-1.23434) | -1 | -1 |
| G: -6289.12860 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.43926 HOMO: -6.57155 LUMO: -0.43538 factor:1 | 1 (-0.94497) | -1 | -1 |
| G: -6289.12860 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.39200 HOMO: -6.72665 LUMO: -0.55239 factor:1 | 1 (-0.89770) | -1 | -1 |
| G: -6289.12860 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.64134 HOMO: -7.05319 LUMO: -1.08573 factor:1 | 1 (-1.14704) | -1 | -1 |
| G: -6289.12860 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.34030 HOMO: -6.56067 LUMO: -0.45715 factor:1 | 1 (-0.84600) | -1 | -1 |
| G: -6289.12860 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.58479 HOMO: -6.76475 LUMO: -0.53879 factor:1 | 1 (-1.09050) | -1 | -1 |
| G: -6289.12860 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.62939 HOMO: -6.67223 LUMO: -0.45987 factor:1 | 1 (-1.13510) | -1 | -1 |
| G: -6289.12860 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.41983 HOMO: -6.44094 LUMO: -0.72110 factor:1 | 1 (-0.92554) | -1 | -1 |
| G: -6289.12860 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.28323 HOMO: -6.66951 LUMO: -0.67756 factor:1 | 1 (-0.78894) | -1 | -1 |
| G: -6289.12860 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.36514 HOMO: -6.69400 LUMO: -0.62858 factor:1 | 1 (-0.87085) | -1 | -1 |
| G: -6289.12860 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.48258 HOMO: -6.51985 LUMO: -0.37007 factor:1 | 1 (-0.98829) | -1 | -1 |
| G: -6289.12860 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.52792 HOMO: -5.98378 LUMO: 0.78641 factor:1 | 1 (-1.03362) | -1 | -1 |
| G: -6289.12860 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.32729 HOMO: -6.11440 LUMO: 0.71294 factor:1 | 1 (-0.83299) | -1 | -1 |
| G: -6289.12860 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.14002 HOMO: -6.45182 LUMO: 0.63947 factor:1 | 1 (-0.64573) | -1 | -1 |
| G: -6289.12860 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12553.86426 HOMO: -6.78924 LUMO: 0.37007 factor:1 | 1 (-0.36997) | -1 | -1 |
| G: -6289.12860 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.39219 HOMO: -6.63686 LUMO: 0.54423 factor:1 | 1 (-0.89789) | -1 | -1 |
| G: -6289.12860 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.37025 HOMO: -6.66679 LUMO: 0.48708 factor:1 | 1 (-1.87595) | -1 | -1 |
| G: -6289.12860 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.39411 HOMO: -6.81917 LUMO: 0.31021 factor:1 | 1 (-1.89982) | -1 | -1 |
| G: -6289.12860 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.37863 HOMO: -6.28583 LUMO: 0.44899 factor:1 | 1 (-1.88433) | -1 | -1 |
| G: -6289.12860 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.95620 HOMO: -6.61237 LUMO: 0.49525 factor:1 | 1 (-1.46190) | -1 | -1 |
| G: -6289.12860 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.18173 HOMO: -7.08857 LUMO: 0.38368 factor:1 | 1 (-1.68743) | -1 | -1 |
| G: -6289.12860 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.09231 HOMO: -6.53890 LUMO: -0.68845 factor:1 | 1 (-1.59802) | -1 | -1 |
| G: -6289.12860 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.16377 HOMO: -6.56611 LUMO: -0.66396 factor:1 | 1 (-1.66947) | -1 | -1 |
| G: -6289.12860 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.60196 HOMO: -6.04909 LUMO: -0.59865 factor:1 | 1 (-1.10767) | -1 | -1 |
| G: -6289.12860 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.35189 HOMO: -6.74842 LUMO: -0.77825 factor:1 | 1 (-0.85759) | -1 | -1 |
| G: -6289.12860 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.38612 HOMO: -6.82462 LUMO: -0.61498 factor:1 | 1 (-0.89183) | -1 | -1 |
| G: -6289.12860 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.20595 HOMO: -7.40694 LUMO: 0.32926 factor:1 | 1 (-0.71166) | -1 | -1 |
| G: -6289.12860 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.16097 HOMO: -6.80557 LUMO: -0.57416 factor:1 | 1 (-0.66668) | -1 | -1 |
| G: -6289.12860 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.10116 HOMO: -6.76747 LUMO: -0.67484 factor:1 | 1 (-0.60687) | -1 | -1 |
| G: -6289.12860 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12553.93531 HOMO: -7.23279 LUMO: 0.48980 factor:1 | 1 (-0.44101) | -1 | -1 |
| G: -6289.12860 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.35110 HOMO: -6.62869 LUMO: -0.24762 factor:1 | 1 (-0.85680) | -1 | -1 |
| G: -6289.12860 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.32440 HOMO: -6.65863 LUMO: -0.28028 factor:1 | 1 (-0.83011) | -1 | -1 |
| G: -6289.12860 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.20744 HOMO: -6.50352 LUMO: -0.44899 factor:1 | 1 (-1.71315) | -1 | -1 |
| G: -6289.12860 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.05487 HOMO: -6.62053 LUMO: -0.88437 factor:1 | 1 (-1.56057) | -1 | -1 |
| G: -6289.12860 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.49463 HOMO: -6.73754 LUMO: -0.77825 factor:1 | 1 (-2.00034) | -1 | -1 |
| G: -6289.12860 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.84360 HOMO: -7.24639 LUMO: 0.35647 factor:1 | 1 (-1.34930) | -1 | -1 |
| G: -6289.12860 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.88308 HOMO: -6.46270 LUMO: -0.48164 factor:1 | 1 (-1.38879) | -1 | -1 |
| G: -6289.12860 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.97971 HOMO: -6.14161 LUMO: -0.66396 factor:1 | 1 (-1.48542) | -1 | -1 |
| G: -6289.12860 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.00752 HOMO: -6.63414 LUMO: 1.51295 factor:1 | 1 (-1.51323) | -1 | -1 |
| G: -6289.12860 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.14012 HOMO: -6.52529 LUMO: 1.65989 factor:1 | 1 (-1.64583) | -1 | -1 |
| G: -6289.12860 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.13383 HOMO: -6.63686 LUMO: 1.64629 factor:1 | 1 (-1.63954) | -1 | -1 |
| G: -6289.12860 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.04123 HOMO: -6.49808 LUMO: 1.60003 factor:1 | 1 (-1.54694) | -1 | -1 |
| G: -6289.12860 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.98518 HOMO: -6.85183 LUMO: 1.96194 factor:1 | 1 (-1.49088) | -1 | -1 |
| G: -6289.12860 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.75995 HOMO: -6.90081 LUMO: 1.82316 factor:1 | 1 (-1.26566) | -1 | -1 |
| G: -6289.12860 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.87633 HOMO: -6.20147 LUMO: 1.95106 factor:1 | 1 (-1.38204) | -1 | -1 |
| G: -6289.12860 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.93152 HOMO: -7.05047 LUMO: 1.94289 factor:1 | 1 (-1.43722) | -1 | -1 |
| G: -6289.12860 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.22355 HOMO: -6.11440 LUMO: 1.83949 factor:1 | 1 (-1.72926) | -1 | -1 |
| G: -6289.12860 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.00306 HOMO: -6.65046 LUMO: 1.59187 factor:1 | 1 (-1.50876) | -1 | -1 |
| G: -6289.12860 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.05166 HOMO: -6.81917 LUMO: 2.41365 factor:1 | 1 (-1.55736) | -1 | -1 |
| G: -6289.12860 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.29898 HOMO: -6.40284 LUMO: 2.48984 factor:1 | 1 (-1.80469) | -1 | -1 |
| G: -6289.12860 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12556.42110 HOMO: -7.04775 LUMO: 2.31025 factor:1 | 1 (-2.92680) | -1 | -1 |
| G: -6289.12860 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.79624 HOMO: -6.64774 LUMO: 2.20140 factor:1 | 1 (-2.30195) | -1 | -1 |
| G: -6289.12860 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12556.57737 HOMO: -6.72393 LUMO: 2.28304 factor:1 | 1 (-3.08308) | -1 | -1 |
| G: -6289.12860 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.59235 HOMO: -6.35114 LUMO: 1.84765 factor:1 | 1 (-2.09805) | -1 | -1 |
| G: -6289.12860 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.61006 HOMO: -6.41100 LUMO: 1.74697 factor:1 | 1 (-2.11577) | -1 | -1 |
| G: -6289.12860 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12556.43644 HOMO: -6.34297 LUMO: 1.55921 factor:1 | 1 (-2.94215) | -1 | -1 |
| G: -6289.12860 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12556.39827 HOMO: -6.31848 LUMO: 1.67622 factor:1 | 1 (-2.90397) | -1 | -1 |
| G: -6289.12860 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12556.01633 HOMO: -6.50896 LUMO: 2.02725 factor:1 | 1 (-2.52203) | -1 | -1 |
| G: -6289.12860 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12556.39759 HOMO: -6.28583 LUMO: 2.00548 factor:1 | 1 (-2.90329) | -1 | -1 |
| G: -6289.12860 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12556.20077 HOMO: -6.67495 LUMO: 1.92384 factor:1 | 1 (-2.70647) | -1 | -1 |
| G: -6289.12860 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.41242 HOMO: -6.17154 LUMO: 2.39732 factor:1 | 1 (-1.91813) | -1 | -1 |
| G: -6289.12860 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.98346 HOMO: -6.84911 LUMO: 2.24766 factor:1 | 1 (-1.48917) | -1 | -1 |
| G: -6289.12860 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12556.16076 HOMO: -6.77564 LUMO: 2.38372 factor:1 | 1 (-2.66647) | -1 | -1 |
| G: -6289.12860 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.26867 HOMO: -6.18243 LUMO: 2.40821 factor:1 | 1 (-1.77437) | -1 | -1 |
| G: -6289.12860 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.42004 HOMO: -6.40828 LUMO: 2.22589 factor:1 | 1 (-1.92575) | -1 | -1 |
| G: -6289.12860 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.04847 HOMO: -6.74570 LUMO: 1.88303 factor:1 | 1 (-1.55418) | -1 | -1 |
| G: -6289.12860 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.61213 HOMO: -6.29944 LUMO: 2.05174 factor:1 | 1 (-2.11783) | -1 | -1 |
| G: -6289.12860 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.33278 HOMO: -7.00693 LUMO: 2.16331 factor:1 | 1 (-1.83848) | -1 | -1 |
| G: -6289.12860 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.43545 HOMO: -6.89537 LUMO: 2.19596 factor:1 | 1 (-1.94115) | -1 | -1 |
| G: -6289.12860 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.48143 HOMO: -6.72665 LUMO: 2.03813 factor:1 | 1 (-1.98714) | -1 | -1 |
| G: -6289.12860 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.35574 HOMO: -6.69944 LUMO: 2.36467 factor:1 | 1 (-1.86145) | -1 | -1 |
| G: -6289.12860 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.79926 HOMO: -6.92802 LUMO: 1.72792 factor:1 | 1 (-2.30497) | -1 | -1 |
| G: -6289.12860 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.60688 HOMO: -6.12256 LUMO: 1.85310 factor:1 | 1 (-2.11258) | -1 | -1 |
| G: -6289.12860 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.64473 HOMO: -6.70489 LUMO: 2.20956 factor:1 | 1 (-2.15043) | -1 | -1 |
| G: -6289.12860 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.61575 HOMO: -6.94707 LUMO: 1.81500 factor:1 | 1 (-2.12145) | -1 | -1 |
| G: -6289.12860 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.23956 HOMO: -6.39468 LUMO: 1.79051 factor:1 | 1 (-0.74527) | -1 | -1 |
| G: -6289.12860 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.40013 HOMO: -6.69128 LUMO: 2.03813 factor:1 | 1 (-0.90584) | -1 | -1 |
| G: -6289.12860 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.24974 HOMO: -6.55250 LUMO: 2.00548 factor:1 | 1 (-0.75544) | -1 | -1 |
| G: -6289.12860 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.44525 HOMO: -6.24773 LUMO: 2.09256 factor:1 | 1 (-0.95096) | -1 | -1 |
| G: -6289.12860 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.32143 HOMO: -6.85727 LUMO: 1.70071 factor:1 | 1 (-1.82714) | -1 | -1 |
| G: -6289.12860 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12556.03823 HOMO: -6.71305 LUMO: 1.72520 factor:1 | 1 (-2.54394) | -1 | -1 |
| G: -6289.12860 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.97173 HOMO: -6.81101 LUMO: 2.15514 factor:1 | 1 (-2.47743) | -1 | -1 |
| G: -6289.12860 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.33612 HOMO: -6.93618 LUMO: 1.75513 factor:1 | 1 (-1.84183) | -1 | -1 |
| G: -6289.12860 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.81398 HOMO: -6.63686 LUMO: 2.09800 factor:1 | 1 (-2.31969) | -1 | -1 |
| G: -6289.12860 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.16886 HOMO: -6.98244 LUMO: 1.72520 factor:1 | 1 (-1.67456) | -1 | -1 |
| G: -6289.12860 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.36393 HOMO: -6.37019 LUMO: 2.35923 factor:1 | 1 (-1.86964) | -1 | -1 |
| G: -6289.12860 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.28576 HOMO: -6.55794 LUMO: 2.12521 factor:1 | 1 (-1.79146) | -1 | -1 |
| G: -6289.12860 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.25599 HOMO: -6.45998 LUMO: 1.93201 factor:1 | 1 (-1.76169) | -1 | -1 |
| G: -6289.12860 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.29974 HOMO: -6.71033 LUMO: 1.58370 factor:1 | 1 (-1.80545) | -1 | -1 |
| G: -6289.12860 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.93582 HOMO: -6.67223 LUMO: 1.52928 factor:1 | 1 (-1.44152) | -1 | -1 |
| G: -6289.12860 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.07421 HOMO: -6.72121 LUMO: 1.33608 factor:1 | 1 (-1.57992) | -1 | -1 |
| G: -6289.12860 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.04017 HOMO: -6.89264 LUMO: 2.08983 factor:1 | 1 (-1.54588) | -1 | -1 |
| G: -6289.12860 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.86632 HOMO: -6.31032 LUMO: 2.24766 factor:1 | 1 (-1.37203) | -1 | -1 |
| G: -6289.12860 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.26083 HOMO: -6.79740 LUMO: 2.09528 factor:1 | 1 (-1.76654) | -1 | -1 |
| G: -6289.12860 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.38555 HOMO: -6.78108 LUMO: 2.15786 factor:1 | 1 (-0.89125) | -1 | -1 |
| G: -6289.12860 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.45328 HOMO: -6.50896 LUMO: 2.15786 factor:1 | 1 (-0.95898) | -1 | -1 |
| G: -6289.12860 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.25058 HOMO: -6.56067 LUMO: 2.24494 factor:1 | 1 (-0.75629) | -1 | -1 |
| G: -6289.12860 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.45698 HOMO: -6.72938 LUMO: 2.24494 factor:1 | 1 (-0.96268) | -1 | -1 |
| G: -6289.12860 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.30566 HOMO: -6.40556 LUMO: 1.58642 factor:1 | 1 (-0.81136) | -1 | -1 |
| G: -6289.12860 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.44824 HOMO: -6.63141 LUMO: 1.66262 factor:1 | 1 (-0.95395) | -1 | -1 |
| G: -6289.12860 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.22242 HOMO: -6.97156 LUMO: 2.23678 factor:1 | 1 (-0.72812) | -1 | -1 |
| G: -6289.12860 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.42819 HOMO: -6.86271 LUMO: 1.91296 factor:1 | 1 (-0.93389) | -1 | -1 |
| G: -6289.12860 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.32177 HOMO: -6.50624 LUMO: 1.89119 factor:1 | 1 (-0.82747) | -1 | -1 |
| G: -6289.12860 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.26503 HOMO: -6.70761 LUMO: 1.56193 factor:1 | 1 (-0.77074) | -1 | -1 |
| G: -6289.12860 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.46318 HOMO: -6.60420 LUMO: 1.79595 factor:1 | 1 (-0.96889) | -1 | -1 |
| G: -6289.12860 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.29115 HOMO: -6.85727 LUMO: 2.26943 factor:1 | 1 (-0.79686) | -1 | -1 |
| G: -6289.12860 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.26315 HOMO: -6.23413 LUMO: 1.91024 factor:1 | 1 (-0.76886) | -1 | -1 |
| G: -6289.12860 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.31172 HOMO: -6.84366 LUMO: 2.01364 factor:1 | 1 (-0.81743) | -1 | -1 |
| G: -6289.12860 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.23423 HOMO: -6.63414 LUMO: 2.54971 factor:1 | 1 (-0.73993) | -1 | -1 |
| G: -6289.12860 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.36865 HOMO: -6.52257 LUMO: 2.42998 factor:1 | 1 (-0.87436) | -1 | -1 |
| G: -6289.12860 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.31276 HOMO: -6.61509 LUMO: 2.31297 factor:1 | 1 (-0.81846) | -1 | -1 |
| G: -6289.12860 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.51565 HOMO: -6.45998 LUMO: 2.23405 factor:1 | 1 (-1.02135) | -1 | -1 |
| G: -6289.12860 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.41026 HOMO: -6.86271 LUMO: 2.22317 factor:1 | 1 (-0.91596) | -1 | -1 |
| G: -6289.12860 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.28922 HOMO: -6.84366 LUMO: 2.11432 factor:1 | 1 (-0.79493) | -1 | -1 |
| G: -6289.12860 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12553.97528 HOMO: -6.85999 LUMO: 2.44902 factor:1 | 1 (-0.48099) | -1 | -1 |
| G: -6289.12860 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.20859 HOMO: -6.73482 LUMO: 1.93745 factor:1 | 1 (-0.71430) | -1 | -1 |
| G: -6289.12860 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.40326 HOMO: -6.91441 LUMO: 2.32385 factor:1 | 1 (-0.90897) | -1 | -1 |
| G: -6289.12860 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.19643 HOMO: -6.16066 LUMO: 2.26399 factor:1 | 1 (-0.70214) | -1 | -1 |
| G: -6289.12860 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.41047 HOMO: -6.71305 LUMO: 2.38644 factor:1 | 1 (-0.91618) | -1 | -1 |
| G: -6289.12860 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.32620 HOMO: -7.08312 LUMO: 2.01636 factor:1 | 1 (-0.83191) | 1 | 1 |
| G: -6289.12860 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.23409 HOMO: -6.15249 LUMO: 1.90752 factor:1 | 1 (-0.73980) | -1 | -1 |
| G: -6289.12860 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.43760 HOMO: -6.83006 LUMO: 2.25855 factor:1 | 1 (-0.94331) | -1 | -1 |
| G: -6289.12860 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.50642 HOMO: -6.77836 LUMO: 2.24766 factor:1 | 1 (-1.01213) | -1 | -1 |
| G: -6289.12860 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.96665 HOMO: -6.66951 LUMO: 2.35923 factor:1 | 1 (-1.47235) | -1 | -1 |
| G: -6289.12860 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.04978 HOMO: -6.68312 LUMO: 2.30208 factor:1 | 1 (-1.55548) | -1 | -1 |
| G: -6289.12860 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.90112 HOMO: -6.49808 LUMO: 2.49801 factor:1 | 1 (-1.40683) | -1 | -1 |
| G: -6289.12860 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.00159 HOMO: -6.62325 LUMO: 1.89935 factor:1 | 1 (-1.50729) | -1 | -1 |
| G: -6289.12860 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.08730 HOMO: -6.80829 LUMO: 1.91296 factor:1 | 1 (-1.59301) | -1 | -1 |
| G: -6289.12860 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.22344 HOMO: -6.64230 LUMO: 2.13065 factor:1 | 1 (-1.72915) | -1 | -1 |
| G: -6289.12860 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.36336 HOMO: -6.40556 LUMO: 1.83949 factor:1 | 1 (-1.86907) | -1 | -1 |
| G: -6289.12860 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.96719 HOMO: -6.48175 LUMO: 1.72248 factor:1 | 1 (-1.47290) | -1 | -1 |
| G: -6289.12860 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.45822 HOMO: -6.61781 LUMO: 2.11432 factor:1 | 1 (-1.96393) | -1 | -1 |
| G: -6289.12860 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12556.38678 HOMO: -6.34570 LUMO: 2.22317 factor:1 | 1 (-2.89249) | -1 | -1 |
| G: -6289.12860 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12556.16795 HOMO: -7.00149 LUMO: 1.80139 factor:1 | 1 (-2.67365) | -1 | -1 |
| G: -6289.12860 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12556.42335 HOMO: -6.66951 LUMO: 2.13065 factor:1 | 1 (-2.92906) | -1 | -1 |
| G: -6289.12860 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.50184 HOMO: -6.54434 LUMO: 2.20140 factor:1 | 1 (-2.00755) | -1 | -1 |
| G: -6289.12860 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12556.01902 HOMO: -6.67767 LUMO: 2.02997 factor:1 | 1 (-2.52473) | -1 | -1 |
| G: -6289.12860 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.41030 HOMO: -6.49536 LUMO: 2.42998 factor:1 | 1 (-1.91601) | -1 | -1 |
| G: -6289.12860 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12556.20528 HOMO: -6.70761 LUMO: 2.71025 factor:1 | 1 (-2.71099) | -1 | -1 |
| G: -6289.12860 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12556.26485 HOMO: -6.62869 LUMO: 2.11160 factor:1 | 1 (-2.77055) | -1 | -1 |
| G: -6289.12860 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.24129 HOMO: -6.61781 LUMO: 2.24494 factor:1 | 1 (-1.74700) | -1 | -1 |
| G: -6289.12860 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12556.05448 HOMO: -6.66135 LUMO: 2.20956 factor:1 | 1 (-2.56018) | -1 | -1 |
| G: -6289.12860 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.45700 HOMO: -6.95523 LUMO: 2.03813 factor:1 | 1 (-1.96270) | -1 | -1 |
| G: -6289.12860 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.27988 HOMO: -7.11578 LUMO: 2.41365 factor:1 | 1 (-1.78558) | 1 | 1 |
| G: -6289.12860 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.18823 HOMO: -6.99061 LUMO: 2.13881 factor:1 | 1 (-1.69394) | -1 | -1 |
| G: -6289.12860 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.34099 HOMO: -6.43277 LUMO: 2.01364 factor:1 | 1 (-1.84670) | -1 | -1 |
| G: -6289.12860 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.40932 HOMO: -6.79196 LUMO: 2.04358 factor:1 | 1 (-1.91503) | -1 | -1 |
| G: -6289.12860 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.26045 HOMO: -7.08584 LUMO: 1.99732 factor:1 | 1 (-1.76616) | 1 | 1 |
| G: -6289.12860 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.96940 HOMO: -6.46815 LUMO: 2.29936 factor:1 | 1 (-1.47510) | -1 | -1 |
| G: -6289.12860 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.46758 HOMO: -6.78108 LUMO: 1.93745 factor:1 | 1 (-1.97329) | -1 | -1 |
| G: -6289.12860 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.38114 HOMO: -6.43277 LUMO: 1.80956 factor:1 | 1 (-0.88685) | -1 | -1 |
| G: -6289.12860 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.39728 HOMO: -6.71577 LUMO: -0.81090 factor:1 | 1 (-0.90298) | -1 | -1 |
| G: -6289.12860 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.35328 HOMO: -7.14027 LUMO: -0.68028 factor:1 | 1 (-0.85898) | -1 | -1 |
| G: -6289.12860 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12553.98236 HOMO: -7.03414 LUMO: -0.69661 factor:1 | 1 (-0.48806) | -1 | -1 |
| G: -6289.12860 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.16582 HOMO: -6.64502 LUMO: -0.47348 factor:1 | 1 (-0.67152) | -1 | -1 |
| G: -6289.12860 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.25055 HOMO: -6.60692 LUMO: 2.12793 factor:1 | 1 (-0.75626) | -1 | -1 |
| G: -6289.12860 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12553.91675 HOMO: -6.66407 LUMO: 1.94561 factor:1 | 1 (-0.42246) | -1 | -1 |
| G: -6289.12860 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.11776 HOMO: -7.10217 LUMO: 1.92384 factor:1 | 1 (-0.62347) | 1 | 1 |
| G: -6289.12860 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.27458 HOMO: -6.84094 LUMO: 1.66534 factor:1 | 1 (-0.78029) | -1 | -1 |
| G: -6289.12860 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.17681 HOMO: -6.93618 LUMO: 2.13065 factor:1 | 1 (-0.68252) | -1 | -1 |
| G: -6289.12860 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.62326 HOMO: -6.60692 LUMO: 2.20684 factor:1 | 1 (-2.12896) | -1 | -1 |
| G: -6289.12860 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.35580 HOMO: -6.85727 LUMO: 2.19324 factor:1 | 1 (-1.86150) | -1 | -1 |
| G: -6289.12860 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12556.39514 HOMO: -6.31032 LUMO: 1.76330 factor:1 | 1 (-2.90084) | -1 | -1 |
| G: -6289.12860 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12556.30681 HOMO: -6.43821 LUMO: 2.10072 factor:1 | 1 (-2.81251) | -1 | -1 |
| G: -6289.12860 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12556.17853 HOMO: -6.42189 LUMO: 2.19596 factor:1 | 1 (-2.68424) | -1 | -1 |
| G: -6289.12860 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.19373 HOMO: -6.40556 LUMO: 2.02181 factor:1 | 1 (-1.69943) | -1 | -1 |
| G: -6289.12860 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12553.87792 HOMO: -6.41372 LUMO: 2.26671 factor:1 | 1 (-0.38363) | -1 | -1 |
| G: -6289.12860 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.09156 HOMO: -6.60692 LUMO: 2.09800 factor:1 | 1 (-0.59726) | -1 | -1 |
| G: -6289.12860 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.24691 HOMO: -6.75931 LUMO: 1.76602 factor:1 | 1 (-0.75261) | -1 | -1 |
| G: -6289.12860 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.83445 HOMO: -6.39195 LUMO: 1.84221 factor:1 | 1 (-2.34015) | -1 | -1 |
| G: -6289.12860 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.80266 HOMO: -6.74570 LUMO: 2.04085 factor:1 | 1 (-2.30837) | -1 | -1 |
| G: -6289.12860 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.00401 HOMO: -6.77019 LUMO: 2.16875 factor:1 | 1 (-1.50971) | -1 | -1 |
| G: -6289.12860 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.69183 HOMO: -6.15522 LUMO: 1.81772 factor:1 | 1 (-2.19754) | -1 | -1 |
| G: -6289.12860 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.87652 HOMO: -6.48175 LUMO: 2.02453 factor:1 | 1 (-1.38223) | -1 | -1 |
| G: -6289.12860 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.90262 HOMO: -6.57427 LUMO: 1.77962 factor:1 | 1 (-1.40833) | -1 | -1 |
| G: -6289.12860 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.88136 HOMO: -6.57699 LUMO: 2.42998 factor:1 | 1 (-2.38706) | -1 | -1 |
| G: -6289.12860 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.09870 HOMO: -6.35386 LUMO: 2.25310 factor:1 | 1 (-1.60441) | -1 | -1 |
| G: -6289.12860 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.11990 HOMO: -6.80013 LUMO: 2.11160 factor:1 | 1 (-1.62561) | -1 | -1 |
| G: -6289.12860 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.23016 HOMO: -6.24229 LUMO: 2.05718 factor:1 | 1 (-1.73587) | -1 | -1 |
| G: -6289.51193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.24925 HOMO: -6.42733 LUMO: 1.76874 factor:1 | 1 (-0.37163) | -1 | -1 |
| G: -6289.51193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.74863 HOMO: -6.56883 LUMO: 2.36195 factor:1 | 1 (-0.87101) | -1 | -1 |
| G: -6289.51193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12556.64135 HOMO: -6.72665 LUMO: 2.28848 factor:1 | 1 (-2.76372) | -1 | -1 |
| G: -6289.51193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12556.08155 HOMO: -6.39195 LUMO: 1.79051 factor:1 | 1 (-2.20393) | -1 | -1 |
| G: -6289.51193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.70810 HOMO: -6.70761 LUMO: 0.15510 factor:1 | 1 (-1.83048) | -1 | -1 |
| G: -6289.51193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.66202 HOMO: -6.44366 LUMO: -0.16871 factor:1 | 1 (-0.78440) | -1 | -1 |
| G: -6289.51193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.40056 HOMO: -6.68584 LUMO: 1.69527 factor:1 | 1 (-1.52294) | -1 | -1 |
| G: -6289.51193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.48611 HOMO: -6.26950 LUMO: 1.61636 factor:1 | 1 (-1.60849) | -1 | -1 |
| G: -6289.51193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12556.10906 HOMO: -6.47631 LUMO: 1.98915 factor:1 | 1 (-2.23144) | -1 | -1 |
| G: -6289.51193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.41662 HOMO: -6.58243 LUMO: 1.97283 factor:1 | 1 (-1.53899) | -1 | -1 |
| G: -6289.51193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.97246 HOMO: -6.51713 LUMO: 1.97283 factor:1 | 1 (-2.09484) | -1 | -1 |
| G: -6289.51193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12556.00275 HOMO: -6.65046 LUMO: 1.69255 factor:1 | 1 (-2.12513) | -1 | -1 |
| G: -6289.51193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.69451 HOMO: -6.26406 LUMO: 2.21773 factor:1 | 1 (-0.81689) | -1 | -1 |
| G: -6289.51193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12556.08310 HOMO: -6.88992 LUMO: 2.28304 factor:1 | 1 (-2.20548) | -1 | -1 |
| G: -6289.51193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.54884 HOMO: -6.67767 LUMO: 2.34834 factor:1 | 1 (-1.67121) | -1 | -1 |
| G: -6289.51193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.59148 HOMO: -6.52801 LUMO: 2.10344 factor:1 | 1 (-1.71385) | -1 | -1 |
| G: -6289.51193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.59877 HOMO: -6.52801 LUMO: 2.24222 factor:1 | 1 (-1.72115) | -1 | -1 |
| G: -6289.51193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.65365 HOMO: -6.17154 LUMO: 1.89663 factor:1 | 1 (-1.77603) | -1 | -1 |
| G: -6289.51193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.71919 HOMO: -6.42733 LUMO: 2.15514 factor:1 | 1 (-0.84157) | -1 | -1 |
| G: -6289.51193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.70757 HOMO: -6.36474 LUMO: 2.01364 factor:1 | 1 (-0.82995) | -1 | -1 |
| G: -6289.51193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.61769 HOMO: -6.82189 LUMO: 1.86942 factor:1 | 1 (-0.74007) | -1 | -1 |
| G: -6289.51193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.72281 HOMO: -6.60148 LUMO: 2.00548 factor:1 | 1 (-0.84519) | -1 | -1 |
| G: -6289.51193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.70787 HOMO: -6.67767 LUMO: 2.15786 factor:1 | 1 (-0.83025) | -1 | -1 |
| G: -6289.51193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.46174 HOMO: -6.79196 LUMO: 2.06534 factor:1 | 1 (-0.58412) | -1 | -1 |
| G: -6289.51193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12556.68480 HOMO: -6.70216 LUMO: 1.83405 factor:1 | 1 (-2.80718) | -1 | -1 |
| G: -6289.51193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.88345 HOMO: -6.58788 LUMO: 1.79051 factor:1 | 1 (-2.00583) | -1 | -1 |
| G: -6289.51193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.54762 HOMO: -6.34842 LUMO: 1.80139 factor:1 | 1 (-0.67000) | -1 | -1 |
| G: -6289.51193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.96054 HOMO: -6.48175 LUMO: 1.95922 factor:1 | 1 (-2.08292) | -1 | -1 |
| G: -6289.51193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12556.01973 HOMO: -6.71033 LUMO: 2.02997 factor:1 | 1 (-2.14211) | -1 | -1 |
| G: -6289.51193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.38168 HOMO: -6.89264 LUMO: 2.42726 factor:1 | 1 (-1.50405) | -1 | -1 |
| G: -6289.51193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.54633 HOMO: -6.74570 LUMO: 2.20684 factor:1 | 1 (-1.66871) | -1 | -1 |
| G: -6289.51193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.49572 HOMO: -6.30216 LUMO: 2.15242 factor:1 | 1 (-1.61810) | -1 | -1 |
| G: -6289.51193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.54122 HOMO: -6.94979 LUMO: 2.43814 factor:1 | 1 (-0.66360) | -1 | -1 |
| G: -6289.51193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.57461 HOMO: -6.97972 LUMO: 2.11432 factor:1 | 1 (-0.69699) | -1 | -1 |
| G: -6289.51193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.67320 HOMO: -6.17154 LUMO: 1.98099 factor:1 | 1 (-0.79558) | -1 | -1 |
| G: -6289.51193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.86651 HOMO: -6.74026 LUMO: 2.21501 factor:1 | 1 (-0.98889) | -1 | -1 |
| G: -6289.51193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.87571 HOMO: -6.72393 LUMO: 2.19596 factor:1 | 1 (-0.99809) | -1 | -1 |
| G: -6289.51193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.81622 HOMO: -6.11440 LUMO: 2.10072 factor:1 | 1 (-0.93860) | -1 | -1 |
| G: -6289.51193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.97568 HOMO: -6.34297 LUMO: 1.92657 factor:1 | 1 (-1.09806) | -1 | -1 |
| G: -6289.51193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.78226 HOMO: -6.24773 LUMO: 2.00276 factor:1 | 1 (-0.90464) | -1 | -1 |
| G: -6289.51193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.38744 HOMO: -6.75114 LUMO: 1.98643 factor:1 | 1 (-1.50982) | -1 | -1 |
| G: -6289.51193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.52130 HOMO: -6.69128 LUMO: 2.08711 factor:1 | 1 (-1.64368) | -1 | -1 |
| G: -6289.51193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.29925 HOMO: -6.65318 LUMO: 2.15514 factor:1 | 1 (-1.42163) | -1 | -1 |
| G: -6289.51193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.67130 HOMO: -6.67495 LUMO: 1.72248 factor:1 | 1 (-0.79367) | -1 | -1 |
| G: -6289.51193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.65012 HOMO: -6.58243 LUMO: 1.83405 factor:1 | 1 (-0.77250) | -1 | -1 |
| G: -6289.51193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.82164 HOMO: -6.61237 LUMO: 1.69799 factor:1 | 1 (-0.94402) | -1 | -1 |
| G: -6289.51193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.69924 HOMO: -6.57427 LUMO: 2.29936 factor:1 | 1 (-0.82162) | -1 | -1 |
| G: -6289.51193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.75658 HOMO: -6.40012 LUMO: 2.35378 factor:1 | 1 (-0.87895) | -1 | -1 |
| G: -6289.51193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.69048 HOMO: -6.90081 LUMO: 2.26671 factor:1 | 1 (-0.81286) | -1 | -1 |
| G: -6289.51193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.39765 HOMO: -6.44910 LUMO: 2.25855 factor:1 | 1 (-1.52003) | -1 | -1 |
| G: -6289.51193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.60682 HOMO: -6.61509 LUMO: 2.26943 factor:1 | 1 (-1.72920) | -1 | -1 |
| G: -6289.51193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.54734 HOMO: -6.78924 LUMO: 2.09256 factor:1 | 1 (-1.66972) | -1 | -1 |
| G: -6289.51193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.77078 HOMO: -6.47087 LUMO: 1.97555 factor:1 | 1 (-0.89316) | -1 | -1 |
| G: -6289.51193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.25792 HOMO: -6.75931 LUMO: 1.98643 factor:1 | 1 (-1.38030) | -1 | -1 |
| G: -6289.51193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.38347 HOMO: -6.17971 LUMO: 2.09800 factor:1 | 1 (-1.50585) | -1 | -1 |
| G: -6289.51193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.34524 HOMO: -6.83006 LUMO: 1.91840 factor:1 | 1 (-1.46762) | -1 | -1 |
| G: -6289.51193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.41803 HOMO: -6.72938 LUMO: 2.17419 factor:1 | 1 (-1.54041) | -1 | -1 |
| G: -6289.51193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.18524 HOMO: -6.78924 LUMO: 2.42726 factor:1 | 1 (-1.30762) | -1 | -1 |
| G: -6289.51193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.19827 HOMO: -6.41372 LUMO: 1.93745 factor:1 | 1 (-1.32065) | -1 | -1 |
| G: -6289.51193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.47436 HOMO: -6.85455 LUMO: 2.14970 factor:1 | 1 (-1.59674) | -1 | -1 |
| G: -6289.51193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12556.70061 HOMO: -6.38651 LUMO: 2.18507 factor:1 | 1 (-2.82299) | -1 | -1 |
| G: -6289.51193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.93363 HOMO: -6.81373 LUMO: 2.00548 factor:1 | 1 (-2.05601) | -1 | -1 |
| G: -6289.51193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.71648 HOMO: -6.64774 LUMO: 2.41365 factor:1 | 1 (-1.83886) | -1 | -1 |
| G: -6289.51193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12556.07206 HOMO: -6.70489 LUMO: 2.31569 factor:1 | 1 (-2.19444) | -1 | -1 |
| G: -6289.51193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.70281 HOMO: -6.49264 LUMO: 1.78779 factor:1 | 1 (-0.82519) | -1 | -1 |
| G: -6289.51193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12556.21807 HOMO: -6.81101 LUMO: 1.86670 factor:1 | 1 (-2.34045) | -1 | -1 |
| G: -6289.51193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.67232 HOMO: -6.72121 LUMO: 1.48846 factor:1 | 1 (-1.79470) | -1 | -1 |
| G: -6289.51193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.76468 HOMO: -6.35930 LUMO: 1.78507 factor:1 | 1 (-0.88706) | -1 | -1 |
| G: -6289.51193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.61064 HOMO: -6.38651 LUMO: 2.04358 factor:1 | 1 (-0.73302) | -1 | -1 |
| G: -6289.51193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.39020 HOMO: -6.42189 LUMO: 1.99187 factor:1 | 1 (-0.51258) | -1 | -1 |
| G: -6289.51193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.53635 HOMO: -6.69400 LUMO: 1.61091 factor:1 | 1 (-0.65873) | -1 | -1 |
| G: -6289.51193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.68678 HOMO: -6.81101 LUMO: 2.17419 factor:1 | 1 (-0.80916) | -1 | -1 |
| G: -6289.51193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.26336 HOMO: -6.90897 LUMO: 2.28576 factor:1 | 1 (-1.38574) | -1 | -1 |
| G: -6289.51193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.31811 HOMO: -6.75387 LUMO: 2.31297 factor:1 | 1 (-1.44049) | -1 | -1 |
| G: -6289.51193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.49142 HOMO: -7.05863 LUMO: 2.18780 factor:1 | 1 (-1.61380) | -1 | -1 |
| G: -6289.51193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.65447 HOMO: -6.56611 LUMO: 1.99187 factor:1 | 1 (-1.77685) | -1 | -1 |
| G: -6289.51193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.40562 HOMO: -6.59060 LUMO: 1.86398 factor:1 | 1 (-1.52800) | -1 | -1 |
| G: -6289.51193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.35355 HOMO: -6.59060 LUMO: 1.59459 factor:1 | 1 (-0.47593) | -1 | -1 |
| G: -6289.51193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.34291 HOMO: -6.57699 LUMO: 1.48030 factor:1 | 1 (-0.46529) | -1 | -1 |
| G: -6289.51193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12556.55971 HOMO: -6.99605 LUMO: 2.30208 factor:1 | 1 (-2.68209) | -1 | -1 |
| G: -6289.51193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.65673 HOMO: -6.42189 LUMO: 2.20412 factor:1 | 1 (-1.77911) | -1 | -1 |
| G: -6289.51193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.31529 HOMO: -7.15115 LUMO: 1.83405 factor:1 | 1 (-0.43767) | 1 | 1 |
| G: -6289.51193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.92762 HOMO: -7.08040 LUMO: 2.21773 factor:1 | 1 (-2.05000) | 1 | 1 |
| G: -6289.51193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12556.04014 HOMO: -6.72121 LUMO: 1.89663 factor:1 | 1 (-2.16252) | -1 | -1 |
| G: -6289.51193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.26508 HOMO: -6.25590 LUMO: 1.85037 factor:1 | 1 (-1.38745) | -1 | -1 |
| G: -6289.51193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.28399 HOMO: -6.70489 LUMO: 1.98915 factor:1 | 1 (-1.40637) | -1 | -1 |
| G: -6289.51193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.66449 HOMO: -6.53617 LUMO: 2.08439 factor:1 | 1 (-0.78687) | -1 | -1 |
| G: -6289.51193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.76854 HOMO: -6.69944 LUMO: 1.98915 factor:1 | 1 (-1.89092) | -1 | -1 |
| G: -6289.51193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.67120 HOMO: -6.79468 LUMO: 1.96466 factor:1 | 1 (-1.79358) | -1 | -1 |
| G: -6289.51193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12556.20950 HOMO: -6.79468 LUMO: 1.99459 factor:1 | 1 (-2.33188) | -1 | -1 |
| G: -6289.51193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.89138 HOMO: -6.58788 LUMO: 1.98371 factor:1 | 1 (-1.01376) | -1 | -1 |
| G: -6289.51193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.41596 HOMO: -6.58788 LUMO: 2.16603 factor:1 | 1 (-1.53834) | -1 | -1 |
| G: -6289.51193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.24475 HOMO: -6.56883 LUMO: 1.64085 factor:1 | 1 (-1.36713) | -1 | -1 |
| G: -6289.51193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.00872 HOMO: -7.19197 LUMO: 2.66127 factor:1 | 1 (-1.13110) | 1 | 1 |
| G: -6289.51193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.95936 HOMO: -6.48175 LUMO: 2.40004 factor:1 | 1 (-1.08173) | -1 | -1 |
| G: -6289.51193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.92877 HOMO: -6.18515 LUMO: 2.27759 factor:1 | 1 (-1.05115) | -1 | -1 |
| G: -6289.51193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.12213 HOMO: -6.64774 LUMO: 2.13337 factor:1 | 1 (-1.24451) | -1 | -1 |
| G: -6289.51193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.97280 HOMO: -6.39740 LUMO: 1.95106 factor:1 | 1 (-1.09518) | -1 | -1 |
| G: -6289.51193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.79601 HOMO: -6.59332 LUMO: 1.81772 factor:1 | 1 (-0.91838) | -1 | -1 |
| G: -6289.51193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.84499 HOMO: -6.68312 LUMO: 2.41909 factor:1 | 1 (-0.96736) | -1 | -1 |
| G: -6289.51193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.54622 HOMO: -5.87494 LUMO: 2.18235 factor:1 | 1 (-1.66860) | -1 | -1 |
| G: -6289.51193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.50007 HOMO: -6.30488 LUMO: 2.04902 factor:1 | 1 (-1.62245) | -1 | -1 |
| G: -6289.51193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.36304 HOMO: -6.65046 LUMO: 2.05446 factor:1 | 1 (-1.48542) | -1 | -1 |
| G: -6289.51193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.65281 HOMO: -6.55794 LUMO: 2.06807 factor:1 | 1 (-1.77519) | -1 | -1 |
| G: -6289.51193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.49479 HOMO: -6.68040 LUMO: 1.99187 factor:1 | 1 (-1.61717) | -1 | -1 |
| G: -6289.51193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.53417 HOMO: -6.60965 LUMO: 2.18780 factor:1 | 1 (-1.65655) | -1 | -1 |
| G: -6289.51193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.63851 HOMO: -6.88176 LUMO: 2.10344 factor:1 | 1 (-0.76088) | -1 | -1 |
| G: -6289.51193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.46551 HOMO: -6.63414 LUMO: 1.70615 factor:1 | 1 (-1.58789) | -1 | -1 |
| G: -6289.51193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.61232 HOMO: -7.15115 LUMO: 2.07351 factor:1 | 1 (-1.73470) | 1 | 1 |
| G: -6289.51193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.45950 HOMO: -6.85727 LUMO: 2.27759 factor:1 | 1 (-1.58188) | -1 | -1 |
| G: -6289.51193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.42383 HOMO: -6.91713 LUMO: 2.28848 factor:1 | 1 (-1.54621) | -1 | -1 |
| G: -6289.51193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.69110 HOMO: -7.10217 LUMO: 2.14698 factor:1 | 1 (-1.81348) | 1 | 1 |
| G: -6289.51193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.57724 HOMO: -6.78108 LUMO: 2.45447 factor:1 | 1 (-1.69962) | -1 | -1 |
| G: -6289.51193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.68906 HOMO: -6.78380 LUMO: 2.43542 factor:1 | 1 (-1.81143) | -1 | -1 |
| G: -6289.51193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.50249 HOMO: -6.60965 LUMO: 2.33474 factor:1 | 1 (-1.62487) | -1 | -1 |
| G: -6289.51193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.61806 HOMO: -6.72665 LUMO: 2.25855 factor:1 | 1 (-1.74044) | -1 | -1 |
| G: -6289.51193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.42007 HOMO: -6.27495 LUMO: 2.04358 factor:1 | 1 (-1.54245) | -1 | -1 |
| G: -6289.51193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.34780 HOMO: -6.17426 LUMO: 1.45853 factor:1 | 1 (-1.47018) | -1 | -1 |
| G: -6289.51193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.72836 HOMO: -7.21374 LUMO: 2.33474 factor:1 | 1 (-0.85074) | 1 | 1 |
| G: -6289.51193 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.44113 HOMO: -6.94707 LUMO: 1.81772 factor:1 | 1 (-1.56351) | -1 | -1 |
| G: -6289.51193 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.36889 HOMO: -6.80829 LUMO: 0.17960 factor:1 | 1 (-1.49127) | -1 | -1 |
| G: -6289.51193 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.38940 HOMO: -7.19469 LUMO: 1.60819 factor:1 | 1 (-1.51178) | 1 | 1 |
| G: -6289.51193 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.48356 HOMO: -6.78652 LUMO: 0.53334 factor:1 | 1 (-1.60593) | -1 | -1 |
| G: -6289.51193 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.59907 HOMO: -6.70489 LUMO: 0.74559 factor:1 | 1 (-1.72145) | -1 | -1 |
| G: -6289.51193 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.71172 HOMO: -6.72393 LUMO: 0.88981 factor:1 | 1 (-1.83410) | -1 | -1 |
| G: -6289.51193 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.87701 HOMO: -4.54430 LUMO: -0.90614 factor:1 | 1 (-0.99939) | -1 | -1 |
| G: -6289.51193 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.32080 HOMO: -6.83006 LUMO: 0.47348 factor:1 | 1 (-1.44318) | -1 | -1 |
| G: -6289.51193 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.98714 HOMO: -7.07496 LUMO: 0.50613 factor:1 | 1 (-1.10952) | -1 | -1 |
| G: -6289.51193 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.27427 HOMO: -6.62053 LUMO: 0.74559 factor:1 | 1 (-1.39665) | -1 | -1 |
| G: -6289.51193 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.02586 HOMO: -6.79196 LUMO: 1.80139 factor:1 | 1 (-1.14824) | -1 | -1 |
| G: -6289.51193 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.39237 HOMO: -6.71033 LUMO: 0.40817 factor:1 | 1 (-1.51475) | -1 | -1 |
| G: -6289.51193 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.46897 HOMO: -6.74026 LUMO: 0.95784 factor:1 | 1 (-1.59135) | -1 | -1 |
| G: -6289.51193 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.46252 HOMO: -7.34707 LUMO: 0.40001 factor:1 | 1 (-1.58490) | -1 | -1 |
| G: -6289.51193 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.44023 HOMO: -6.19875 LUMO: -0.88709 factor:1 | 1 (-1.56261) | -1 | -1 |
| G: -6289.51193 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.04311 HOMO: -6.48719 LUMO: -0.14694 factor:1 | 1 (-1.16549) | -1 | -1 |
| G: -6289.51193 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.00779 HOMO: -6.73482 LUMO: -0.01633 factor:1 | 1 (-1.13017) | -1 | -1 |
| G: -6289.51193 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.26616 HOMO: -7.05591 LUMO: -0.20136 factor:1 | 1 (-1.38854) | -1 | -1 |
| G: -6289.51193 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.14711 HOMO: -6.38651 LUMO: -2.07895 factor:1 | 1 (-1.26949) | -1 | -1 |
| G: -6289.51193 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.10635 HOMO: -6.85455 LUMO: -1.03403 factor:1 | 1 (-1.22873) | -1 | -1 |
| G: -6289.51193 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.73323 HOMO: -6.72121 LUMO: -0.99322 factor:1 | 1 (-0.85561) | -1 | -1 |
| G: -6289.51193 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.92801 HOMO: -6.53890 LUMO: -0.10885 factor:1 | 1 (-1.05039) | -1 | -1 |
| G: -6289.51193 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.91440 HOMO: -6.68312 LUMO: 0.21225 factor:1 | 1 (-1.03678) | -1 | -1 |
| G: -6289.51193 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.85573 HOMO: -6.68040 LUMO: 0.21225 factor:1 | 1 (-0.97811) | -1 | -1 |
| G: -6289.51193 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.48422 HOMO: -6.76475 LUMO: -0.64491 factor:1 | 1 (-0.60660) | -1 | -1 |
| G: -6289.51193 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.99331 HOMO: -6.48175 LUMO: 0.41633 factor:1 | 1 (-1.11569) | -1 | -1 |
| G: -6289.51193 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.62117 HOMO: -6.42733 LUMO: 0.16599 factor:1 | 1 (-0.74355) | -1 | -1 |
| G: -6289.51193 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.35904 HOMO: -6.66679 LUMO: 0.77825 factor:1 | 1 (-1.48142) | -1 | -1 |
| G: -6289.51193 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.89507 HOMO: -6.75931 LUMO: -0.73471 factor:1 | 1 (-2.01745) | -1 | -1 |
| G: -6289.51193 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.85657 HOMO: -6.53617 LUMO: 0.38096 factor:1 | 1 (-1.97895) | -1 | -1 |
| G: -6289.51193 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12556.42352 HOMO: -6.34297 LUMO: 0.35375 factor:1 | 1 (-2.54590) | -1 | -1 |
| G: -6289.51193 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12556.25546 HOMO: -7.11850 LUMO: -0.03265 factor:1 | 1 (-2.37784) | -1 | -1 |
| G: -6289.51193 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.93594 HOMO: -5.21914 LUMO: 1.29798 factor:1 | 1 (-2.05832) | -1 | -1 |
| G: -6289.51193 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.54247 HOMO: -7.09129 LUMO: -0.66668 factor:1 | 1 (-1.66485) | -1 | -1 |
| G: -6289.51193 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.85921 HOMO: -6.96884 LUMO: -0.31021 factor:1 | 1 (-1.98159) | -1 | -1 |
| G: -6289.51193 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.81126 HOMO: -6.51713 LUMO: -0.59865 factor:1 | 1 (-1.93364) | -1 | -1 |
| G: -6289.51193 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12556.06357 HOMO: -6.69400 LUMO: -0.07075 factor:1 | 1 (-2.18595) | -1 | -1 |
| G: -6289.51193 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12556.39748 HOMO: -5.28173 LUMO: 1.17281 factor:1 | 1 (-2.51986) | -1 | -1 |
| G: -6289.51193 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12556.39677 HOMO: -6.54434 LUMO: 0.32109 factor:1 | 1 (-2.51915) | -1 | -1 |
| G: -6289.51193 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12556.55440 HOMO: -6.79740 LUMO: -0.24762 factor:1 | 1 (-2.67678) | -1 | -1 |
| G: -6289.51193 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.91496 HOMO: -6.91986 LUMO: -0.14694 factor:1 | 1 (-2.03734) | -1 | -1 |
| G: -6289.51193 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12556.60692 HOMO: -6.75114 LUMO: 0.18504 factor:1 | 1 (-2.72930) | -1 | -1 |
| G: -6289.51193 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12556.45731 HOMO: -6.74842 LUMO: 0.69389 factor:1 | 1 (-2.57969) | -1 | -1 |
| G: -6289.51193 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.65442 HOMO: -7.01782 LUMO: 0.56600 factor:1 | 1 (-1.77679) | -1 | -1 |
| G: -6289.51193 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.88794 HOMO: -6.47359 LUMO: -0.56600 factor:1 | 1 (-2.01032) | -1 | -1 |
| G: -6289.51193 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12556.57098 HOMO: -6.63686 LUMO: -0.55783 factor:1 | 1 (-2.69336) | -1 | -1 |
| G: -6289.51193 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12556.44131 HOMO: -4.13885 LUMO: -2.05446 factor:1 | 1 (-2.56369) | -1 | -1 |
| G: -6289.51193 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12556.10923 HOMO: -6.34570 LUMO: 0.19864 factor:1 | 1 (-2.23161) | -1 | -1 |
| G: -6289.51193 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.84634 HOMO: -6.47903 LUMO: 0.24762 factor:1 | 1 (-1.96872) | -1 | -1 |
| G: -6289.51193 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.55694 HOMO: -6.15249 LUMO: 0.32109 factor:1 | 1 (-1.67932) | -1 | -1 |
| G: -6289.51193 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.41551 HOMO: -6.84366 LUMO: 0.29116 factor:1 | 1 (-0.53789) | -1 | -1 |
| G: -6289.51193 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.28005 HOMO: -6.34297 LUMO: 0.19864 factor:1 | 1 (-0.40243) | -1 | -1 |
| G: -6289.51193 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.44350 HOMO: -6.51168 LUMO: 0.30749 factor:1 | 1 (-1.56588) | -1 | -1 |
| G: -6289.51193 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.49281 HOMO: -6.79468 LUMO: -0.16599 factor:1 | 1 (-1.61519) | -1 | -1 |
| G: -6289.51193 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.68609 HOMO: -7.24095 LUMO: 0.15238 factor:1 | 1 (-1.80847) | -1 | -1 |
| G: -6289.51193 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.37958 HOMO: -7.06952 LUMO: -0.34558 factor:1 | 1 (-1.50196) | -1 | -1 |
| G: -6289.51193 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.79856 HOMO: -6.88176 LUMO: 0.02177 factor:1 | 1 (-0.92094) | -1 | -1 |
| G: -6289.51193 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.65685 HOMO: -6.37291 LUMO: -0.69117 factor:1 | 1 (-0.77923) | -1 | -1 |
| G: -6289.51193 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.57687 HOMO: -6.83278 LUMO: -0.59049 factor:1 | 1 (-0.69925) | -1 | -1 |
| G: -6289.51193 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.75309 HOMO: -6.57155 LUMO: -0.33470 factor:1 | 1 (-0.87547) | -1 | -1 |
| G: -6289.51193 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.74934 HOMO: -6.89537 LUMO: -0.58504 factor:1 | 1 (-0.87172) | -1 | -1 |
| G: -6289.51193 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.45328 HOMO: -6.57155 LUMO: -0.34831 factor:1 | 1 (-0.57566) | -1 | -1 |
| G: -6289.51193 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12556.04680 HOMO: -6.64774 LUMO: -0.95784 factor:1 | 1 (-2.16918) | -1 | -1 |
| G: -6289.51193 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12556.48874 HOMO: -6.91713 LUMO: -0.69933 factor:1 | 1 (-2.61112) | -1 | -1 |
| G: -6289.51193 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.55527 HOMO: -6.80557 LUMO: -0.65035 factor:1 | 1 (-0.67765) | -1 | -1 |
| G: -6289.51193 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.89015 HOMO: -7.26544 LUMO: -0.79729 factor:1 | 1 (-2.01253) | -1 | -1 |
| G: -6289.51193 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.23318 HOMO: -6.69128 LUMO: -0.16871 factor:1 | 1 (-1.35556) | -1 | -1 |
| G: -6289.51193 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.55499 HOMO: -6.88448 LUMO: 0.13061 factor:1 | 1 (-1.67736) | -1 | -1 |
| G: -6289.51193 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12556.12569 HOMO: -6.50352 LUMO: 0.12245 factor:1 | 1 (-2.24807) | -1 | -1 |
| G: -6289.51193 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.77570 HOMO: -6.56067 LUMO: 0.17687 factor:1 | 1 (-1.89808) | -1 | -1 |
| G: -6289.51193 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.51722 HOMO: -6.70216 LUMO: 0.25034 factor:1 | 1 (-1.63959) | -1 | -1 |
| G: -6289.51193 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.43194 HOMO: -6.51713 LUMO: -0.78369 factor:1 | 1 (-1.55431) | -1 | -1 |
| G: -6289.51193 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.58217 HOMO: -6.50352 LUMO: 0.12245 factor:1 | 1 (-1.70455) | -1 | -1 |
| G: -6289.51193 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.21248 HOMO: -6.22052 LUMO: -0.83811 factor:1 | 1 (-1.33485) | -1 | -1 |
| G: -6289.51193 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.55833 HOMO: -6.51168 LUMO: -0.76464 factor:1 | 1 (-1.68071) | -1 | -1 |
| G: -6289.51193 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.85545 HOMO: -7.14571 LUMO: -0.80274 factor:1 | 1 (-1.97783) | -1 | -1 |
| G: -6289.51193 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.42883 HOMO: -6.66679 LUMO: -0.88709 factor:1 | 1 (-1.55121) | -1 | -1 |
| G: -6289.51193 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.27749 HOMO: -6.76203 LUMO: -1.43948 factor:1 | 1 (-0.39987) | -1 | -1 |
| G: -6289.51193 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.46408 HOMO: -6.57427 LUMO: -1.62996 factor:1 | 1 (-0.58646) | -1 | -1 |
| G: -6289.51193 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12553.99694 HOMO: -5.05043 LUMO: 1.24900 factor:1 | 1 (-0.11932) | -1 | -1 |
| G: -6289.51193 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.56631 HOMO: -6.53345 LUMO: 0.23130 factor:1 | 1 (-0.68869) | -1 | -1 |
| G: -6289.51193 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.33210 HOMO: -7.18381 LUMO: -0.22585 factor:1 | 1 (-1.45448) | -1 | -1 |
| G: -6289.51193 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.94101 HOMO: -7.00965 LUMO: -1.79595 factor:1 | 1 (-2.06338) | -1 | -1 |
| G: -6289.51193 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.48211 HOMO: -6.08174 LUMO: -0.82995 factor:1 | 1 (-1.60449) | -1 | -1 |
| G: -6289.51193 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.18861 HOMO: -6.42189 LUMO: -0.84355 factor:1 | 1 (-1.31099) | -1 | -1 |
| G: -6289.51193 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.86854 HOMO: -6.53890 LUMO: 0.60409 factor:1 | 1 (-1.99092) | -1 | -1 |
| G: -6289.51193 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.79665 HOMO: -6.62869 LUMO: 0.43810 factor:1 | 1 (-1.91903) | -1 | -1 |
| G: -6289.51193 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.95600 HOMO: -6.68312 LUMO: 0.64491 factor:1 | 1 (-2.07838) | -1 | -1 |
| G: -6289.51193 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.59431 HOMO: -6.42189 LUMO: 1.51295 factor:1 | 1 (-1.71668) | -1 | -1 |
| G: -6289.51193 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.42780 HOMO: -6.17971 LUMO: 1.67622 factor:1 | 1 (-1.55018) | -1 | -1 |
| G: -6289.51193 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.37030 HOMO: -6.79196 LUMO: 1.36873 factor:1 | 1 (-1.49268) | -1 | -1 |
| G: -6289.51193 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.71711 HOMO: -7.38517 LUMO: 0.56328 factor:1 | 1 (-1.83949) | 1 | 1 |
| G: -6289.51193 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.42543 HOMO: -7.56204 LUMO: 0.71566 factor:1 | 1 (-1.54781) | 1 | 1 |
| G: -6289.51193 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.78242 HOMO: -6.45726 LUMO: -1.91840 factor:1 | 1 (-1.90480) | -1 | -1 |
| G: -6289.51193 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.82971 HOMO: -6.13073 LUMO: -0.97417 factor:1 | 1 (-1.95209) | -1 | -1 |
| G: -6289.51193 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.97521 HOMO: -6.50352 LUMO: -0.69661 factor:1 | 1 (-2.09759) | -1 | -1 |
| G: -6289.51193 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.66103 HOMO: -6.76747 LUMO: -1.71976 factor:1 | 1 (-1.78341) | -1 | -1 |
| G: -6289.51193 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.51219 HOMO: -6.48447 LUMO: -0.89525 factor:1 | 1 (-0.63457) | -1 | -1 |
| G: -6289.51193 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.43222 HOMO: -7.11850 LUMO: -0.71566 factor:1 | 1 (-0.55460) | -1 | -1 |
| G: -6289.51193 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.61187 HOMO: -6.80285 LUMO: -0.49253 factor:1 | 1 (-0.73424) | -1 | -1 |
| G: -6289.51193 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.32040 HOMO: -6.80557 LUMO: -0.88165 factor:1 | 1 (-0.44278) | -1 | -1 |
| G: -6289.51193 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.59978 HOMO: -6.94162 LUMO: -0.08980 factor:1 | 1 (-0.72216) | -1 | -1 |
| G: -6289.51193 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.40179 HOMO: -6.97972 LUMO: -0.29388 factor:1 | 1 (-1.52416) | -1 | -1 |
| G: -6289.51193 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.97271 HOMO: -6.75114 LUMO: 0.04626 factor:1 | 1 (-2.09509) | -1 | -1 |
| G: -6289.51193 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.34627 HOMO: -7.15932 LUMO: 0.68845 factor:1 | 1 (-1.46865) | 1 | 1 |
| G: -6289.51193 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12556.20109 HOMO: -7.36612 LUMO: 0.63675 factor:1 | 1 (-2.32347) | 1 | 1 |
| G: -6289.51193 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.54625 HOMO: -7.02598 LUMO: -0.66124 factor:1 | 1 (-1.66863) | -1 | -1 |
| G: -6289.51193 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.88593 HOMO: -6.89264 LUMO: -0.54967 factor:1 | 1 (-2.00831) | -1 | -1 |
| G: -6289.51193 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.32987 HOMO: -6.97700 LUMO: 0.27756 factor:1 | 1 (-1.45224) | -1 | -1 |
| G: -6289.51193 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.18616 HOMO: -6.60965 LUMO: 0.08163 factor:1 | 1 (-1.30854) | -1 | -1 |
| G: -6289.51193 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.41874 HOMO: -6.70761 LUMO: 0.40001 factor:1 | 1 (-1.54112) | -1 | -1 |
| G: -6289.51193 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.47463 HOMO: -6.69128 LUMO: 0.23674 factor:1 | 1 (-1.59701) | -1 | -1 |
| G: -6289.51193 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.20216 HOMO: -6.69128 LUMO: -0.69933 factor:1 | 1 (-1.32454) | -1 | -1 |
| G: -6289.51193 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.10755 HOMO: -6.18515 LUMO: -0.85988 factor:1 | 1 (-1.22993) | -1 | -1 |
| G: -6289.51193 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.89584 HOMO: -6.86815 LUMO: -1.90208 factor:1 | 1 (-1.01822) | -1 | -1 |
| G: -6289.51193 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.05076 HOMO: -6.37563 LUMO: -1.74697 factor:1 | 1 (-1.17314) | -1 | -1 |
| G: -6289.51193 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.35009 HOMO: -6.75659 LUMO: 0.36463 factor:1 | 1 (-0.47247) | -1 | -1 |
| G: -6289.51193 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.53429 HOMO: -6.91441 LUMO: -0.88981 factor:1 | 1 (-0.65667) | -1 | -1 |
| G: -6289.51193 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.68240 HOMO: -6.71305 LUMO: -0.29933 factor:1 | 1 (-0.80478) | -1 | -1 |
| G: -6289.51193 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.84537 HOMO: -6.91441 LUMO: -1.04492 factor:1 | 1 (-0.96775) | -1 | -1 |
| G: -6289.51193 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.72025 HOMO: -6.05453 LUMO: -0.83539 factor:1 | 1 (-0.84263) | -1 | -1 |
| G: -6289.51193 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.33523 HOMO: -7.35252 LUMO: -0.45715 factor:1 | 1 (-0.45761) | -1 | -1 |
| G: -6289.51193 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.41393 HOMO: -6.41644 LUMO: -0.97417 factor:1 | 1 (-0.53631) | -1 | -1 |
| G: -6289.51193 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.74822 HOMO: -6.78924 LUMO: 0.36735 factor:1 | 1 (-0.87060) | -1 | -1 |
| G: -6289.51193 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.38854 HOMO: -6.74298 LUMO: 0.51974 factor:1 | 1 (-0.51092) | -1 | -1 |
| G: -6289.51193 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.62724 HOMO: -6.48992 LUMO: 1.44765 factor:1 | 1 (-0.74962) | -1 | -1 |
| G: -6289.51193 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.29366 HOMO: -6.12528 LUMO: 1.57826 factor:1 | 1 (-0.41603) | -1 | -1 |
| G: -6289.51193 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.77864 HOMO: -6.62325 LUMO: 1.57826 factor:1 | 1 (-0.90102) | -1 | -1 |
| G: -6289.51193 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.46397 HOMO: -6.19875 LUMO: 1.29798 factor:1 | 1 (-0.58635) | -1 | -1 |
| G: -6289.51193 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.63271 HOMO: -6.74570 LUMO: 1.52112 factor:1 | 1 (-0.75509) | -1 | -1 |
| G: -6289.51193 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.62936 HOMO: -6.84094 LUMO: 1.48574 factor:1 | 1 (-0.75174) | -1 | -1 |
| G: -6289.51193 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.30228 HOMO: -6.85183 LUMO: 0.33470 factor:1 | 1 (-0.42466) | -1 | -1 |
| G: -6289.51193 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.20144 HOMO: -6.51168 LUMO: 0.48164 factor:1 | 1 (-0.32382) | -1 | -1 |
| G: -6289.51193 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.38955 HOMO: -6.25046 LUMO: 0.75648 factor:1 | 1 (-0.51193) | -1 | -1 |
| G: -6289.51193 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.42691 HOMO: -6.65591 LUMO: 0.32109 factor:1 | 1 (-0.54929) | -1 | -1 |
| G: -6289.51193 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.53001 HOMO: -6.71033 LUMO: 0.40817 factor:1 | 1 (-0.65239) | -1 | -1 |
| G: -6289.51193 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.44019 HOMO: -6.75114 LUMO: 0.73471 factor:1 | 1 (-0.56257) | -1 | -1 |
| G: -6289.51193 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.25118 HOMO: -6.50624 LUMO: 0.59321 factor:1 | 1 (-0.37356) | -1 | -1 |
| G: -6289.51193 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.74692 HOMO: -6.39740 LUMO: 0.83267 factor:1 | 1 (-0.86929) | -1 | -1 |
| G: -6289.51193 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.66773 HOMO: -6.44094 LUMO: 0.65579 factor:1 | 1 (-0.79011) | -1 | -1 |
| G: -6289.51193 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.80055 HOMO: -6.52257 LUMO: 0.05714 factor:1 | 1 (-0.92293) | -1 | -1 |
| G: -6289.51193 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.66735 HOMO: -7.10217 LUMO: 0.49797 factor:1 | 1 (-0.78973) | -1 | -1 |
| G: -6289.51193 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.41320 HOMO: -6.83006 LUMO: 0.55783 factor:1 | 1 (-0.53557) | -1 | -1 |
| G: -6289.51193 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.52378 HOMO: -6.99333 LUMO: -0.79457 factor:1 | 1 (-0.64616) | -1 | -1 |
| G: -6289.51193 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.56373 HOMO: -6.64230 LUMO: 0.32382 factor:1 | 1 (-0.68611) | -1 | -1 |
| G: -6289.51193 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.19877 HOMO: -6.90897 LUMO: 0.30749 factor:1 | 1 (-0.32115) | -1 | -1 |
| G: -6289.51193 HOMO: -7.26544 LUMO: -1.10478 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.26500 HOMO: -7.09129 LUMO: 1.33336 factor:1 | 1 (-0.38738) | 1 | 1 |
| G: -6289.51193 HOMO: -7.26544 LUMO: -1.10478 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.42604 HOMO: -6.66951 LUMO: 1.34424 factor:1 | 1 (-0.54842) | -1 | -1 |
| G: -6289.51193 HOMO: -7.26544 LUMO: -1.10478 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.46571 HOMO: -7.02870 LUMO: 1.48574 factor:1 | 1 (-0.58809) | -1 | -1 |
| G: -6289.51193 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.56142 HOMO: -7.26544 LUMO: 0.32926 factor:1 | 1 (-0.68379) | -1 | -1 |
| G: -6289.51193 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.54381 HOMO: -6.56067 LUMO: -0.45987 factor:1 | 1 (-0.66619) | -1 | -1 |
| G: -6289.51193 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.67834 HOMO: -6.54434 LUMO: -0.28300 factor:1 | 1 (-0.80072) | -1 | -1 |
| G: -6289.51193 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.42332 HOMO: -7.19469 LUMO: 0.54695 factor:1 | 1 (-0.54570) | -1 | -1 |
| G: -6289.51193 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.46095 HOMO: -6.47359 LUMO: -0.22041 factor:1 | 1 (-0.58333) | -1 | -1 |
| G: -6289.51193 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.10170 HOMO: -6.80013 LUMO: 2.08167 factor:1 | 1 (-1.22408) | -1 | -1 |
| G: -6289.51193 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.20706 HOMO: -6.23957 LUMO: 1.67894 factor:1 | 1 (-1.32944) | -1 | -1 |
| G: -6289.51193 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.30053 HOMO: -6.75114 LUMO: -0.62858 factor:1 | 1 (-1.42291) | -1 | -1 |
| G: -6289.51193 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.34951 HOMO: -6.79468 LUMO: -0.64491 factor:1 | 1 (-1.47189) | -1 | -1 |
| G: -6289.51193 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.98787 HOMO: -6.84911 LUMO: -0.69661 factor:1 | 1 (-1.11025) | -1 | -1 |
| G: -6289.51193 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.99492 HOMO: -7.54028 LUMO: 0.25851 factor:1 | 1 (-1.11730) | -1 | -1 |
| G: -6289.51193 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.35988 HOMO: -6.92802 LUMO: -0.71022 factor:1 | 1 (-1.48226) | -1 | -1 |
| G: -6289.51193 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.15843 HOMO: -6.72665 LUMO: -0.46804 factor:1 | 1 (-1.28081) | -1 | -1 |
| G: -6289.51193 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.70421 HOMO: -6.63686 LUMO: -0.23674 factor:1 | 1 (-1.82659) | -1 | -1 |
| G: -6289.51193 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.80133 HOMO: -7.21102 LUMO: 0.54423 factor:1 | 1 (-1.92371) | -1 | -1 |
| G: -6289.51193 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12556.57601 HOMO: -6.63414 LUMO: -0.25034 factor:1 | 1 (-2.69839) | -1 | -1 |
| G: -6289.51193 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12556.55519 HOMO: -6.70761 LUMO: -0.31837 factor:1 | 1 (-2.67757) | -1 | -1 |
| G: -6289.51193 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.83722 HOMO: -6.57155 LUMO: 1.76874 factor:1 | 1 (-1.95960) | -1 | -1 |
| G: -6289.51193 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12556.40556 HOMO: -6.84366 LUMO: 2.04358 factor:1 | 1 (-2.52794) | -1 | -1 |
| G: -6289.51193 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12556.27206 HOMO: -6.60420 LUMO: 1.80139 factor:1 | 1 (-2.39444) | -1 | -1 |
| G: -6289.51193 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.60386 HOMO: -7.03686 LUMO: 2.21229 factor:1 | 1 (-1.72624) | -1 | -1 |
| G: -6289.51193 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12556.09045 HOMO: -6.77564 LUMO: 1.97555 factor:1 | 1 (-2.21283) | -1 | -1 |
| G: -6289.51193 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.45866 HOMO: -6.40012 LUMO: 2.17691 factor:1 | 1 (-1.58104) | -1 | -1 |
| G: -6289.51193 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.46579 HOMO: -6.80013 LUMO: 2.25582 factor:1 | 1 (-1.58817) | -1 | -1 |
| G: -6289.51193 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.36274 HOMO: -6.74298 LUMO: 2.31569 factor:1 | 1 (-1.48512) | -1 | -1 |
| G: -6289.51193 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.71178 HOMO: -6.68856 LUMO: 1.85854 factor:1 | 1 (-1.83416) | -1 | -1 |
| G: -6289.51193 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.39857 HOMO: -6.17971 LUMO: 1.52928 factor:1 | 1 (-1.52095) | -1 | -1 |
| G: -6289.51193 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.61440 HOMO: -6.54162 LUMO: 1.91840 factor:1 | 1 (-0.73678) | -1 | -1 |
| G: -6289.51193 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.61851 HOMO: -6.80013 LUMO: -0.55511 factor:1 | 1 (-0.74088) | -1 | -1 |
| G: -6289.51193 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.30334 HOMO: -7.46953 LUMO: 0.28572 factor:1 | 1 (-0.42572) | -1 | -1 |
| G: -6289.51193 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.71309 HOMO: -6.61781 LUMO: -0.54967 factor:1 | 1 (-0.83547) | -1 | -1 |
| G: -6289.51193 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.50000 HOMO: -6.56339 LUMO: -0.47892 factor:1 | 1 (-0.62238) | -1 | -1 |
| G: -6289.51193 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.29050 HOMO: -6.65591 LUMO: -0.25307 factor:1 | 1 (-0.41288) | -1 | -1 |
| G: -6289.51193 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.54531 HOMO: -6.62869 LUMO: -0.23402 factor:1 | 1 (-0.66769) | -1 | -1 |
| G: -6289.51193 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.39230 HOMO: -6.58243 LUMO: -0.19048 factor:1 | 1 (-0.51468) | -1 | -1 |
| G: -6289.51193 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.87047 HOMO: -7.27632 LUMO: 0.52790 factor:1 | 1 (-1.99285) | -1 | -1 |
| G: -6289.51193 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12556.40550 HOMO: -7.21102 LUMO: 0.57688 factor:1 | 1 (-2.52788) | -1 | -1 |
| G: -6289.51193 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.53828 HOMO: -6.72393 LUMO: -0.53879 factor:1 | 1 (-1.66066) | -1 | -1 |
| G: -6289.51193 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12556.52069 HOMO: -7.42054 LUMO: -0.99322 factor:1 | 1 (-2.64307) | -1 | -1 |
| G: -6289.51193 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12556.22874 HOMO: -6.88992 LUMO: -0.71838 factor:1 | 1 (-2.35112) | -1 | -1 |
| G: -6289.51193 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.26968 HOMO: -6.88176 LUMO: -0.61226 factor:1 | 1 (-0.39206) | -1 | -1 |
| G: -6289.51193 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.48653 HOMO: -7.36340 LUMO: -1.04492 factor:1 | 1 (-0.60891) | -1 | -1 |
| G: -6289.51193 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.27308 HOMO: -6.65863 LUMO: -0.41906 factor:1 | 1 (-0.39546) | -1 | -1 |
| G: -6289.51193 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.87967 HOMO: -7.15115 LUMO: -0.66396 factor:1 | 1 (-2.00205) | -1 | -1 |
| G: -6289.51193 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.10967 HOMO: -7.10489 LUMO: -0.64491 factor:1 | 1 (-1.23205) | -1 | -1 |
| G: -6289.51193 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.28453 HOMO: -7.20285 LUMO: 0.47892 factor:1 | 1 (-1.40691) | -1 | -1 |
| G: -6289.51193 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12556.05744 HOMO: -6.55794 LUMO: -0.28844 factor:1 | 1 (-2.17982) | -1 | -1 |
| G: -6289.51193 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.19008 HOMO: -7.19197 LUMO: -0.69661 factor:1 | 1 (-1.31246) | -1 | -1 |
| G: -6289.51193 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.80177 HOMO: -6.56883 LUMO: -0.32926 factor:1 | 1 (-1.92414) | -1 | -1 |
| G: -6289.51193 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.96692 HOMO: -6.70761 LUMO: 1.95650 factor:1 | 1 (-1.08930) | -1 | -1 |
| G: -6289.51193 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.46219 HOMO: -6.60420 LUMO: 1.80684 factor:1 | 1 (-1.58457) | -1 | -1 |
| G: -6289.51193 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.51469 HOMO: -6.84094 LUMO: 1.64085 factor:1 | 1 (-1.63706) | -1 | -1 |
| G: -6289.51193 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.28654 HOMO: -6.69128 LUMO: 1.90208 factor:1 | 1 (-1.40892) | -1 | -1 |
| G: -6289.51193 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.33955 HOMO: -6.75387 LUMO: 1.70343 factor:1 | 1 (-1.46193) | -1 | -1 |
| G: -6289.51193 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.43308 HOMO: -7.07496 LUMO: 2.10072 factor:1 | 1 (-1.55546) | -1 | -1 |
| G: -6289.51193 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.27237 HOMO: -6.99877 LUMO: 2.24494 factor:1 | 1 (-1.39475) | -1 | -1 |
| G: -6289.51193 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.29114 HOMO: -6.63414 LUMO: 2.17691 factor:1 | 1 (-1.41352) | -1 | -1 |
| G: -6289.51193 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.09334 HOMO: -6.44638 LUMO: 1.78235 factor:1 | 1 (-1.21572) | -1 | -1 |
| G: -6289.51193 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.70125 HOMO: -6.87632 LUMO: 1.84221 factor:1 | 1 (-1.82363) | -1 | -1 |
| G: -6289.51193 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.47221 HOMO: -6.85183 LUMO: 1.68711 factor:1 | 1 (-1.59459) | -1 | -1 |
| G: -6289.51193 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.67575 HOMO: -6.96339 LUMO: 2.26671 factor:1 | 1 (-1.79813) | -1 | -1 |
| G: -6289.51193 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12556.24724 HOMO: -6.63141 LUMO: 1.96738 factor:1 | 1 (-2.36962) | -1 | -1 |
| G: -6289.51193 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.42998 HOMO: -6.37019 LUMO: 2.23133 factor:1 | 1 (-1.55236) | -1 | -1 |
| G: -6289.51193 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12556.02416 HOMO: -7.11034 LUMO: 2.32385 factor:1 | 1 (-2.14654) | 1 | 1 |
| G: -6289.51193 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.28502 HOMO: -6.91986 LUMO: 1.65445 factor:1 | 1 (-1.40740) | -1 | -1 |
| G: -6289.51193 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.44636 HOMO: -7.12938 LUMO: 2.28304 factor:1 | 1 (-1.56874) | 1 | 1 |
| G: -6289.51193 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.29955 HOMO: -6.54978 LUMO: 1.92112 factor:1 | 1 (-1.42193) | -1 | -1 |
| G: -6289.51193 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.13996 HOMO: -6.83006 LUMO: 2.48712 factor:1 | 1 (-1.26234) | -1 | -1 |
| G: -6289.51193 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.45069 HOMO: -6.97972 LUMO: 1.96738 factor:1 | 1 (-0.57307) | -1 | -1 |
| G: -6289.51193 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.28729 HOMO: -6.69944 LUMO: 2.06262 factor:1 | 1 (-0.40967) | -1 | -1 |
| G: -6289.51193 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.28609 HOMO: -6.76747 LUMO: 2.10888 factor:1 | 1 (-0.40847) | -1 | -1 |
| G: -6289.51193 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.41619 HOMO: -6.91169 LUMO: 2.06534 factor:1 | 1 (-0.53857) | -1 | -1 |
| G: -6289.51193 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.45989 HOMO: -7.03414 LUMO: 1.93473 factor:1 | 1 (-0.58227) | -1 | -1 |
| G: -6289.51193 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.17227 HOMO: -7.03142 LUMO: 2.52250 factor:1 | 1 (-0.29464) | -1 | -1 |
| G: -6289.51193 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.18378 HOMO: -6.34025 LUMO: 2.61229 factor:1 | 1 (-0.30616) | -1 | -1 |
| G: -6289.51193 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.42408 HOMO: -6.98788 LUMO: 2.28304 factor:1 | 1 (-0.54646) | -1 | -1 |
| G: -6289.51193 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.23956 HOMO: -6.97700 LUMO: 2.53882 factor:1 | 1 (-0.36194) | -1 | -1 |
| G: -6289.51193 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.01452 HOMO: -6.58788 LUMO: 1.94289 factor:1 | 1 (-0.13690) | -1 | -1 |
| G: -6289.51193 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.36002 HOMO: -6.78652 LUMO: 2.13609 factor:1 | 1 (-0.48240) | -1 | -1 |
| G: -6289.51193 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.24974 HOMO: -6.55250 LUMO: 1.82861 factor:1 | 1 (-0.37212) | -1 | -1 |
| G: -6289.51193 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.69458 HOMO: -6.45998 LUMO: 1.75786 factor:1 | 1 (-1.81696) | -1 | -1 |
| G: -6289.51193 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12556.54091 HOMO: -6.78924 LUMO: 2.33746 factor:1 | 1 (-2.66329) | -1 | -1 |
| G: -6289.51193 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.47561 HOMO: -6.85727 LUMO: 1.76058 factor:1 | 1 (-1.59799) | -1 | -1 |
| G: -6289.51193 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.17578 HOMO: -6.70489 LUMO: 1.84493 factor:1 | 1 (-0.29816) | -1 | -1 |
| G: -6289.51193 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.32821 HOMO: -6.71305 LUMO: 1.53472 factor:1 | 1 (-0.45059) | -1 | -1 |
| G: -6289.51193 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.30291 HOMO: -6.76747 LUMO: 1.48846 factor:1 | 1 (-0.42529) | -1 | -1 |
| G: -6289.51193 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.90936 HOMO: -6.69128 LUMO: 1.95922 factor:1 | 1 (-2.03174) | -1 | -1 |
| G: -6289.51193 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.22799 HOMO: -6.67495 LUMO: 2.05446 factor:1 | 1 (-1.35037) | -1 | -1 |
| G: -6289.51193 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.76027 HOMO: -6.63686 LUMO: 2.25310 factor:1 | 1 (-1.88265) | -1 | -1 |
| G: -6289.51193 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.15008 HOMO: -6.63958 LUMO: 2.14154 factor:1 | 1 (-1.27246) | -1 | -1 |
| G: -6289.51193 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.30859 HOMO: -6.62597 LUMO: 2.01908 factor:1 | 1 (-1.43097) | -1 | -1 |
| G: -6289.51193 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12556.02985 HOMO: -7.07768 LUMO: 2.14154 factor:1 | 1 (-2.15223) | -1 | -1 |
| G: -6289.51193 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.39613 HOMO: -6.19603 LUMO: 2.01092 factor:1 | 1 (-1.51850) | -1 | -1 |
| G: -6289.51193 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12556.18607 HOMO: -6.65046 LUMO: 2.15786 factor:1 | 1 (-2.30845) | -1 | -1 |
| G: -6289.51193 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.23756 HOMO: -6.92258 LUMO: 2.31841 factor:1 | 1 (-1.35994) | -1 | -1 |
| G: -6289.51193 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.66379 HOMO: -6.90081 LUMO: 2.19324 factor:1 | 1 (-0.78616) | -1 | -1 |
| G: -6289.51193 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.52811 HOMO: -6.85455 LUMO: 1.95650 factor:1 | 1 (-0.65049) | -1 | -1 |
| G: -6289.51193 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.71554 HOMO: -6.57699 LUMO: 1.76058 factor:1 | 1 (-0.83792) | -1 | -1 |
| G: -6289.51193 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.53162 HOMO: -6.90625 LUMO: 1.97555 factor:1 | 1 (-0.65400) | -1 | -1 |
| G: -6289.51193 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.36748 HOMO: -6.97428 LUMO: 1.92929 factor:1 | 1 (-0.48986) | -1 | -1 |
| G: -6289.51193 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.70226 HOMO: -6.61781 LUMO: -0.41906 factor:1 | 1 (-0.82464) | -1 | -1 |
| G: -6289.51193 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.97987 HOMO: -6.62869 LUMO: -0.81906 factor:1 | 1 (-1.10225) | -1 | -1 |
| G: -6289.51193 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.93024 HOMO: -7.01237 LUMO: 2.00548 factor:1 | 1 (-1.05262) | -1 | -1 |
| G: -6289.51193 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.80942 HOMO: -6.85727 LUMO: 2.17691 factor:1 | 1 (-0.93180) | -1 | -1 |
| G: -6289.51193 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.43570 HOMO: -6.71849 LUMO: 1.58914 factor:1 | 1 (-0.55808) | -1 | -1 |
| G: -6289.51193 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.96667 HOMO: -7.52395 LUMO: 0.27211 factor:1 | 1 (-1.08905) | -1 | -1 |
| G: -6289.51193 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.70354 HOMO: -6.96611 LUMO: -0.72654 factor:1 | 1 (-0.82592) | -1 | -1 |
| G: -6289.51193 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.84681 HOMO: -6.89537 LUMO: -0.68028 factor:1 | 1 (-0.96919) | -1 | -1 |
| G: -6289.51193 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.75056 HOMO: -6.84911 LUMO: -0.58504 factor:1 | 1 (-0.87294) | -1 | -1 |
| G: -6289.51193 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.85497 HOMO: -6.79196 LUMO: -0.55783 factor:1 | 1 (-0.97735) | -1 | -1 |
| G: -6289.51193 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.87220 HOMO: -6.67767 LUMO: 1.79323 factor:1 | 1 (-0.99458) | -1 | -1 |
| G: -6289.51193 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.69236 HOMO: -6.54434 LUMO: 1.91024 factor:1 | 1 (-0.81474) | -1 | -1 |
| G: -6289.51193 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.53344 HOMO: -6.62869 LUMO: 1.69799 factor:1 | 1 (-0.65582) | -1 | -1 |
| G: -6289.51193 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.70104 HOMO: -6.72393 LUMO: 2.12249 factor:1 | 1 (-0.82342) | -1 | -1 |
| G: -6289.51193 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.68400 HOMO: -6.66407 LUMO: 2.05990 factor:1 | 1 (-0.80638) | -1 | -1 |
| G: -6289.51193 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.37143 HOMO: -7.00149 LUMO: 1.82044 factor:1 | 1 (-0.49381) | -1 | -1 |
| G: -6289.51193 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.71546 HOMO: -7.12122 LUMO: 2.16058 factor:1 | 1 (-0.83784) | 1 | 1 |
| G: -6289.51193 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.74888 HOMO: -6.63141 LUMO: 2.21229 factor:1 | 1 (-0.87125) | -1 | -1 |
| G: -6289.51193 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.37329 HOMO: -6.37835 LUMO: 2.32113 factor:1 | 1 (-1.49567) | -1 | -1 |
| G: -6289.51193 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.41319 HOMO: -6.99605 LUMO: 2.00548 factor:1 | 1 (-1.53557) | -1 | -1 |
| G: -6289.51193 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.61496 HOMO: -6.85999 LUMO: 2.39460 factor:1 | 1 (-1.73734) | -1 | -1 |
| G: -6289.51193 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.59529 HOMO: -6.85727 LUMO: 2.48712 factor:1 | 1 (-1.71766) | -1 | -1 |
| G: -6289.51193 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.52426 HOMO: -7.04231 LUMO: 2.40277 factor:1 | 1 (-1.64664) | -1 | -1 |
| G: -6289.51193 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.46176 HOMO: -6.60692 LUMO: 2.26671 factor:1 | 1 (-1.58414) | -1 | -1 |
| G: -6289.51193 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.80063 HOMO: -6.67495 LUMO: 2.14698 factor:1 | 1 (-0.92301) | -1 | -1 |
| G: -6289.51193 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.93165 HOMO: -6.73210 LUMO: 2.06807 factor:1 | 1 (-1.05403) | -1 | -1 |
| G: -6289.51193 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.79171 HOMO: -7.20013 LUMO: 2.02181 factor:1 | 1 (-0.91408) | 1 | 1 |
| G: -6289.51193 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.04488 HOMO: -7.18653 LUMO: 2.29936 factor:1 | 1 (-1.16726) | 1 | 1 |
| G: -6289.51193 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.32366 HOMO: -6.92802 LUMO: 2.36195 factor:1 | 1 (-1.44604) | -1 | -1 |
| G: -6289.51193 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.24480 HOMO: -6.89537 LUMO: 1.78779 factor:1 | 1 (-1.36718) | -1 | -1 |
| G: -6289.51193 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.30709 HOMO: -6.96067 LUMO: 2.31297 factor:1 | 1 (-1.42947) | -1 | -1 |
| G: -6289.51193 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.36823 HOMO: -6.91441 LUMO: 2.50345 factor:1 | 1 (-1.49061) | -1 | -1 |
| G: -6289.51193 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.25479 HOMO: -7.17292 LUMO: 2.12521 factor:1 | 1 (-1.37717) | 1 | 1 |
| G: -6289.51193 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.98858 HOMO: -6.93618 LUMO: 2.35106 factor:1 | 1 (-1.11096) | -1 | -1 |
| G: -6289.51193 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.49531 HOMO: -6.75931 LUMO: 1.61908 factor:1 | 1 (-1.61769) | -1 | -1 |
| G: -6289.51193 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.42979 HOMO: -6.35930 LUMO: 1.23540 factor:1 | 1 (-1.55216) | -1 | -1 |
| G: -6289.51193 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.28491 HOMO: -6.17971 LUMO: 1.84493 factor:1 | 1 (-1.40729) | -1 | -1 |
| G: -6289.51193 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.09043 HOMO: -6.72665 LUMO: 2.61229 factor:1 | 1 (-1.21281) | -1 | -1 |
| G: -6289.51193 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.10589 HOMO: -6.62869 LUMO: 2.28304 factor:1 | 1 (-1.22827) | -1 | -1 |
| G: -6289.51193 HOMO: -8.88180 LUMO: 1.02315 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.33610 HOMO: -6.58243 LUMO: 0.28028 factor:1 | 1 (-1.45848) | -1 | -1 |
| G: -6289.51193 HOMO: -8.88180 LUMO: 1.02315 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.36807 HOMO: -6.79468 LUMO: 0.14966 factor:1 | 1 (-1.49045) | -1 | -1 |
| G: -6289.51193 HOMO: -8.88180 LUMO: 1.02315 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.10679 HOMO: -6.63141 LUMO: 0.31021 factor:1 | 1 (-1.22917) | -1 | -1 |
| G: -6289.51193 HOMO: -8.88180 LUMO: 1.02315 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.94224 HOMO: -6.81101 LUMO: 0.13878 factor:1 | 1 (-1.06462) | -1 | -1 |
| G: -6289.51193 HOMO: -8.88180 LUMO: 1.02315 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.29370 HOMO: -6.72665 LUMO: 0.65579 factor:1 | 1 (-1.41608) | -1 | -1 |
| G: -6289.51193 HOMO: -8.88180 LUMO: 1.02315 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.35142 HOMO: -6.53073 LUMO: 0.91430 factor:1 | 1 (-1.47380) | -1 | -1 |
| G: -6289.51193 HOMO: -8.88180 LUMO: 1.02315 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.63042 HOMO: -7.19197 LUMO: 1.62996 factor:1 | 1 (-0.75280) | 1 | 1 |
| G: -6289.51193 HOMO: -8.88180 LUMO: 1.02315 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.56806 HOMO: -6.69400 LUMO: 0.84627 factor:1 | 1 (-0.69043) | -1 | -1 |
| G: -6289.51193 HOMO: -8.88180 LUMO: 1.02315 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.39341 HOMO: -6.76475 LUMO: 0.51974 factor:1 | 1 (-0.51579) | -1 | -1 |
| G: -6289.51193 HOMO: -8.88180 LUMO: 1.02315 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.21458 HOMO: -6.67767 LUMO: 0.52246 factor:1 | 1 (-0.33696) | -1 | -1 |
| G: -6289.51193 HOMO: -8.88180 LUMO: 1.02315 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.14043 HOMO: -6.73210 LUMO: 0.94424 factor:1 | 1 (-0.26281) | -1 | -1 |
| G: -6289.51193 HOMO: -8.88180 LUMO: 1.02315 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.77296 HOMO: -6.97972 LUMO: 0.60409 factor:1 | 1 (-0.89534) | -1 | -1 |
| G: -6289.51193 HOMO: -8.88180 LUMO: 1.02315 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.45850 HOMO: -7.38517 LUMO: 0.73743 factor:1 | 1 (-0.58088) | -1 | -1 |
| G: -6289.51193 HOMO: -8.88180 LUMO: 1.02315 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.61687 HOMO: -6.48992 LUMO: 1.08301 factor:1 | 1 (-0.73925) | -1 | -1 |
| G: -6289.51193 HOMO: -8.88180 LUMO: 1.02315 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.70006 HOMO: -7.18381 LUMO: 1.61908 factor:1 | 1 (-0.82244) | 1 | 1 |
| G: -6289.51193 HOMO: -8.88180 LUMO: 1.02315 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.50748 HOMO: -6.74842 LUMO: 0.57960 factor:1 | 1 (-0.62986) | -1 | -1 |
| G: -6289.51193 HOMO: -8.88180 LUMO: 1.02315 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.34389 HOMO: -6.67495 LUMO: 0.77280 factor:1 | 1 (-0.46627) | -1 | -1 |
| G: -6289.51193 HOMO: -8.88180 LUMO: 1.02315 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.59108 HOMO: -6.74570 LUMO: 0.77280 factor:1 | 1 (-0.71346) | -1 | -1 |
| G: -6289.51193 HOMO: -8.88180 LUMO: 1.02315 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.49173 HOMO: -6.73754 LUMO: 0.86804 factor:1 | 1 (-0.61411) | -1 | -1 |
| G: -6289.51193 HOMO: -8.88180 LUMO: 1.02315 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.62348 HOMO: -6.66135 LUMO: 0.94424 factor:1 | 1 (-0.74586) | -1 | -1 |
| G: -6289.51193 HOMO: -8.88180 LUMO: 1.02315 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.41907 HOMO: -6.44638 LUMO: 1.00138 factor:1 | 1 (-0.54145) | -1 | -1 |
| G: -6289.51193 HOMO: -8.88180 LUMO: 1.02315 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.27417 HOMO: -6.65591 LUMO: 1.02043 factor:1 | 1 (-0.39655) | -1 | -1 |
| G: -6289.51193 HOMO: -8.88180 LUMO: 1.02315 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.55823 HOMO: -7.17564 LUMO: 0.50069 factor:1 | 1 (-0.68061) | -1 | -1 |
| G: -6289.51193 HOMO: -8.88180 LUMO: 1.02315 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.24412 HOMO: -6.59332 LUMO: 0.79457 factor:1 | 1 (-1.36650) | -1 | -1 |
| G: -6289.51193 HOMO: -8.88180 LUMO: 1.02315 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.28050 HOMO: -6.76747 LUMO: 1.73881 factor:1 | 1 (-1.40288) | -1 | -1 |
| G: -6289.51193 HOMO: -8.88180 LUMO: 1.02315 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.20548 HOMO: -7.00421 LUMO: 1.07485 factor:1 | 1 (-1.32786) | -1 | -1 |
| G: -6289.51193 HOMO: -8.88180 LUMO: 1.02315 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.85255 HOMO: -6.94979 LUMO: 1.67894 factor:1 | 1 (-0.97493) | -1 | -1 |
| G: -6289.51193 HOMO: -8.88180 LUMO: 1.02315 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.27327 HOMO: -6.66135 LUMO: 0.47076 factor:1 | 1 (-1.39564) | -1 | -1 |
| G: -6289.51193 HOMO: -8.88180 LUMO: 1.02315 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.07533 HOMO: -6.74298 LUMO: 1.85037 factor:1 | 1 (-1.19771) | -1 | -1 |
| G: -6289.51193 HOMO: -8.88180 LUMO: 1.02315 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.75056 HOMO: -6.65318 LUMO: 0.95240 factor:1 | 1 (-0.87294) | -1 | -1 |
| G: -6289.51193 HOMO: -8.88180 LUMO: 1.02315 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.52359 HOMO: -6.63958 LUMO: 0.78097 factor:1 | 1 (-0.64597) | -1 | -1 |
| G: -6289.51193 HOMO: -8.88180 LUMO: 1.02315 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.60291 HOMO: -6.11712 LUMO: 0.40001 factor:1 | 1 (-0.72529) | -1 | -1 |
| G: -6289.51193 HOMO: -8.88180 LUMO: 1.02315 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.25371 HOMO: -7.08312 LUMO: 0.92519 factor:1 | 1 (-0.37609) | -1 | -1 |
| G: -6289.51193 HOMO: -8.88180 LUMO: 1.02315 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.67540 HOMO: -6.96067 LUMO: 0.54695 factor:1 | 1 (-0.79778) | -1 | -1 |
| G: -6289.51193 HOMO: -8.88180 LUMO: 1.02315 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.34794 HOMO: -6.74026 LUMO: 0.60137 factor:1 | 1 (-0.47032) | -1 | -1 |
| G: -6289.51193 HOMO: -8.88180 LUMO: 1.02315 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.19618 HOMO: -6.74298 LUMO: 0.59593 factor:1 | 1 (-0.31856) | -1 | -1 |
| G: -6289.51193 HOMO: -8.88180 LUMO: 1.02315 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.47156 HOMO: -6.93074 LUMO: 0.60681 factor:1 | 1 (-0.59394) | -1 | -1 |
| G: -6289.51193 HOMO: -8.88180 LUMO: 1.02315 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.44552 HOMO: -6.41644 LUMO: 0.35919 factor:1 | 1 (-0.56790) | -1 | -1 |
| G: -6289.51193 HOMO: -8.88180 LUMO: 1.02315 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.63059 HOMO: -6.41917 LUMO: 1.73064 factor:1 | 1 (-0.75297) | -1 | -1 |
| G: -6289.51193 HOMO: -8.88180 LUMO: 1.02315 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.74634 HOMO: -4.64226 LUMO: -0.87893 factor:1 | 1 (-0.86872) | -1 | -1 |
| G: -6289.51193 HOMO: -8.88180 LUMO: 1.02315 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.83247 HOMO: -6.59604 LUMO: 0.90342 factor:1 | 1 (-0.95485) | -1 | -1 |
| G: -6289.51193 HOMO: -8.88180 LUMO: 1.02315 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.58528 HOMO: -6.79468 LUMO: 0.50069 factor:1 | 1 (-0.70766) | -1 | -1 |
| G: -6289.51193 HOMO: -8.88180 LUMO: 1.02315 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.54672 HOMO: -7.04503 LUMO: 0.52518 factor:1 | 1 (-0.66910) | -1 | -1 |
| G: -6289.51193 HOMO: -8.88180 LUMO: 1.02315 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.42247 HOMO: -6.69400 LUMO: 0.54423 factor:1 | 1 (-0.54485) | -1 | -1 |
| G: -6289.51193 HOMO: -8.88180 LUMO: 1.02315 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.54158 HOMO: -6.51713 LUMO: 0.95240 factor:1 | 1 (-0.66396) | -1 | -1 |
| G: -6289.51193 HOMO: -8.88180 LUMO: 1.02315 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.55548 HOMO: -6.88176 LUMO: 1.79323 factor:1 | 1 (-0.67786) | -1 | -1 |
| G: -6289.51193 HOMO: -8.88180 LUMO: 1.02315 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.29717 HOMO: -6.71849 LUMO: 0.28844 factor:1 | 1 (-0.41955) | -1 | -1 |
| G: -6289.51193 HOMO: -8.88180 LUMO: 1.02315 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.61508 HOMO: -6.94979 LUMO: 0.51974 factor:1 | 1 (-0.73746) | -1 | -1 |
| G: -6289.51193 HOMO: -8.88180 LUMO: 1.02315 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.26838 HOMO: -6.76203 LUMO: 0.94151 factor:1 | 1 (-0.39076) | -1 | -1 |
| G: -6289.51193 HOMO: -8.88180 LUMO: 1.02315 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.37134 HOMO: -6.91169 LUMO: 0.89525 factor:1 | 1 (-0.49372) | -1 | -1 |
| G: -6289.51193 HOMO: -8.88180 LUMO: 1.02315 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.18625 HOMO: -6.83006 LUMO: 0.89253 factor:1 | 1 (-0.30863) | -1 | -1 |
| G: -6289.51193 HOMO: -8.88180 LUMO: 1.02315 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.00451 HOMO: -7.08857 LUMO: 0.60409 factor:1 | 1 (-0.12689) | -1 | -1 |
| G: -6289.51193 HOMO: -8.88180 LUMO: 1.02315 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.50678 HOMO: -6.91713 LUMO: 1.76330 factor:1 | 1 (-0.62915) | -1 | -1 |
| G: -6289.51193 HOMO: -8.88180 LUMO: 1.02315 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.17507 HOMO: -6.47359 LUMO: 1.56193 factor:1 | 1 (-0.29745) | -1 | -1 |
| G: -6289.51193 HOMO: -6.91169 LUMO: -0.53879 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.76575 HOMO: -7.00149 LUMO: 1.47214 factor:1 | 1 (-0.88813) | -1 | -1 |
| G: -6289.51193 HOMO: -6.91169 LUMO: -0.53879 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.65780 HOMO: -7.03686 LUMO: 1.97283 factor:1 | 1 (-0.78018) | -1 | -1 |
| G: -6289.51193 HOMO: -6.91169 LUMO: -0.53879 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.14975 HOMO: -7.00965 LUMO: 1.64629 factor:1 | 1 (-1.27213) | -1 | -1 |
| G: -6289.51193 HOMO: -6.91169 LUMO: -0.53879 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.18023 HOMO: -7.06952 LUMO: 1.67622 factor:1 | 1 (-1.30261) | 1 | -1 |
| G: -6289.51193 HOMO: -6.91169 LUMO: -0.53879 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.04140 HOMO: -6.80557 LUMO: 1.70615 factor:1 | 1 (-1.16378) | -1 | -1 |
| G: -6289.51193 HOMO: -6.91169 LUMO: -0.53879 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.36113 HOMO: -6.80829 LUMO: 1.71704 factor:1 | 1 (-1.48351) | -1 | -1 |
| G: -6289.51193 HOMO: -6.91169 LUMO: -0.53879 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.41039 HOMO: -7.26544 LUMO: 1.89935 factor:1 | 1 (-0.53277) | 1 | -1 |
| G: -6289.51193 HOMO: -7.29809 LUMO: 2.83543 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.26166 HOMO: -7.00149 LUMO: 1.47214 factor:1 | 1 (-0.38403) | -1 | -1 |
| G: -6289.51193 HOMO: -7.29809 LUMO: 2.83543 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12553.97194 HOMO: -7.03686 LUMO: 1.97283 factor:1 | 1 (-0.09431) | -1 | -1 |
| G: -6289.51193 HOMO: -7.29809 LUMO: 2.83543 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.07330 HOMO: -7.00965 LUMO: 1.64629 factor:1 | 1 (-0.19568) | -1 | -1 |
| G: -6289.51193 HOMO: -7.29809 LUMO: 2.83543 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12553.76902 HOMO: -7.06952 LUMO: 1.67622 factor:1 | -1 (0.10860) | -1 | -1 |
| G: -6289.51193 HOMO: -7.29809 LUMO: 2.83543 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12553.41067 HOMO: -6.80557 LUMO: 1.70615 factor:1 | -1 (0.46695) | -1 | -1 |
| G: -6289.51193 HOMO: -7.29809 LUMO: 2.83543 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.17548 HOMO: -6.80829 LUMO: 1.71704 factor:1 | 1 (-0.29786) | -1 | -1 |
| G: -6289.51193 HOMO: -7.29809 LUMO: 2.83543 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.85171 HOMO: -7.26544 LUMO: 1.89935 factor:1 | 1 (-0.97409) | -1 | -1 |
| G: -6289.51193 HOMO: -7.85865 LUMO: 2.83543 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.72523 HOMO: -7.00149 LUMO: 1.75241 factor:1 | 1 (-0.84761) | -1 | -1 |
| G: -6289.51193 HOMO: -7.85865 LUMO: 2.83543 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.63233 HOMO: -6.91169 LUMO: 2.07079 factor:1 | 1 (-0.75471) | -1 | -1 |
| G: -6289.51193 HOMO: -7.85865 LUMO: 2.83543 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.82349 HOMO: -7.11034 LUMO: 1.76330 factor:1 | 1 (-0.94587) | -1 | -1 |
| G: -6289.51193 HOMO: -7.85865 LUMO: 2.83543 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.54321 HOMO: -6.87360 LUMO: 2.02725 factor:1 | 1 (-0.66559) | -1 | -1 |
| G: -6289.51193 HOMO: -7.85865 LUMO: 2.83543 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.64433 HOMO: -7.08584 LUMO: 1.82044 factor:1 | 1 (-0.76671) | -1 | -1 |
| G: -6289.51193 HOMO: -7.85865 LUMO: 2.83543 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.39890 HOMO: -6.90625 LUMO: 1.68166 factor:1 | 1 (-1.52128) | -1 | -1 |
| G: -6289.51193 HOMO: -7.85865 LUMO: 2.83543 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.51724 HOMO: -6.71577 LUMO: 1.93201 factor:1 | 1 (-1.63962) | -1 | -1 |
| G: -6289.51193 HOMO: -7.85865 LUMO: 2.83543 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.55733 HOMO: -6.99605 LUMO: 2.08439 factor:1 | 1 (-1.67970) | -1 | -1 |
| G: -6289.51193 HOMO: -7.85865 LUMO: 2.83543 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.30592 HOMO: -7.02326 LUMO: 1.97010 factor:1 | 1 (-1.42830) | -1 | -1 |
| G: -6289.51193 HOMO: -7.85865 LUMO: 2.83543 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.35501 HOMO: -6.99877 LUMO: 2.15514 factor:1 | 1 (-1.47739) | -1 | -1 |
| G: -6289.51193 HOMO: -7.85865 LUMO: 2.83543 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.73402 HOMO: -6.75387 LUMO: 1.95106 factor:1 | 1 (-0.85640) | -1 | -1 |
| G: -6289.51193 HOMO: -7.85865 LUMO: 2.83543 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.80036 HOMO: -7.10761 LUMO: 2.06262 factor:1 | 1 (-0.92274) | -1 | -1 |
| G: -6289.51193 HOMO: -7.85865 LUMO: 2.83543 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.63363 HOMO: -7.03142 LUMO: 1.91568 factor:1 | 1 (-0.75601) | -1 | -1 |
| G: -6289.51193 HOMO: -7.85865 LUMO: 2.83543 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.52204 HOMO: -6.98788 LUMO: 1.98371 factor:1 | 1 (-0.64442) | -1 | -1 |
| G: -6289.51193 HOMO: -7.85865 LUMO: 2.83543 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.42841 HOMO: -6.94707 LUMO: 1.68438 factor:1 | 1 (-0.55079) | -1 | -1 |
| G: -6289.51193 HOMO: -7.85865 LUMO: 2.83543 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.35205 HOMO: -6.88176 LUMO: 2.20684 factor:1 | 1 (-0.47443) | -1 | -1 |
| G: -6289.51193 HOMO: -7.85865 LUMO: 2.83543 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.38996 HOMO: -6.73210 LUMO: 2.18780 factor:1 | 1 (-0.51234) | -1 | -1 |
| G: -6289.51193 HOMO: -7.85865 LUMO: 2.83543 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.11594 HOMO: -6.83822 LUMO: 2.06807 factor:1 | 1 (-0.23832) | -1 | -1 |
| G: -6289.51193 HOMO: -7.85865 LUMO: 2.83543 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.48307 HOMO: -6.78924 LUMO: 2.42181 factor:1 | 1 (-0.60545) | -1 | -1 |
| G: -6289.51193 HOMO: -7.85865 LUMO: 2.83543 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.35400 HOMO: -6.94707 LUMO: 1.71704 factor:1 | 1 (-1.47638) | -1 | -1 |
| G: -6289.51193 HOMO: -7.85865 LUMO: 2.83543 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.54952 HOMO: -6.85183 LUMO: 1.78779 factor:1 | 1 (-1.67189) | -1 | -1 |
| G: -6289.51193 HOMO: -7.85865 LUMO: 2.83543 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.08924 HOMO: -6.98788 LUMO: 1.69799 factor:1 | 1 (-1.21161) | -1 | -1 |
| G: -6289.51193 HOMO: -7.85865 LUMO: 2.83543 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.51860 HOMO: -6.79468 LUMO: 2.04358 factor:1 | 1 (-1.64098) | -1 | -1 |
| G: -6289.51193 HOMO: -7.85865 LUMO: 2.83543 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.36355 HOMO: -6.90081 LUMO: 1.97283 factor:1 | 1 (-1.48593) | -1 | -1 |
| G: -6289.51193 HOMO: -7.85865 LUMO: 2.83543 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.80575 HOMO: -6.79468 LUMO: 2.00820 factor:1 | 1 (-0.92813) | -1 | -1 |
| G: -6289.51193 HOMO: -7.85865 LUMO: 2.83543 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.54626 HOMO: -7.06408 LUMO: 2.29936 factor:1 | 1 (-0.66864) | -1 | -1 |
| G: -6289.51193 HOMO: -7.85865 LUMO: 2.83543 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.68245 HOMO: -6.78924 LUMO: 2.13337 factor:1 | 1 (-0.80483) | -1 | -1 |
| G: -6289.51193 HOMO: -7.85865 LUMO: 2.83543 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.37311 HOMO: -6.79468 LUMO: 2.35106 factor:1 | 1 (-0.49549) | -1 | -1 |
| G: -6289.51193 HOMO: -7.85865 LUMO: 2.83543 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.17839 HOMO: -6.82734 LUMO: 2.16603 factor:1 | 1 (-0.30077) | -1 | -1 |
| G: -6289.51193 HOMO: -7.85865 LUMO: 2.83543 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.39826 HOMO: -6.79740 LUMO: 2.36739 factor:1 | 1 (-0.52064) | -1 | -1 |
| G: -6289.51193 HOMO: -7.85865 LUMO: 2.83543 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.60539 HOMO: -7.14027 LUMO: 2.10888 factor:1 | 1 (-0.72777) | -1 | -1 |
| G: -6289.51193 HOMO: -6.61509 LUMO: -0.23674 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.75625 HOMO: -6.96067 LUMO: 1.59731 factor:1 | 1 (-0.87863) | -1 | -1 |
| G: -6289.51193 HOMO: -6.61509 LUMO: -0.23674 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.44792 HOMO: -6.91169 LUMO: 1.37145 factor:1 | 1 (-0.57030) | -1 | -1 |
| G: -6289.51193 HOMO: -6.61509 LUMO: -0.23674 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.55932 HOMO: -6.94707 LUMO: 1.73064 factor:1 | 1 (-0.68170) | -1 | -1 |
| G: -6289.51193 HOMO: -6.61509 LUMO: -0.23674 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.62261 HOMO: -7.02326 LUMO: 1.41227 factor:1 | 1 (-0.74499) | -1 | -1 |
| G: -6289.51193 HOMO: -6.61509 LUMO: -0.23674 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.19605 HOMO: -6.72121 LUMO: 1.43132 factor:1 | 1 (-0.31843) | -1 | -1 |
| G: -6289.51193 HOMO: -6.61509 LUMO: -0.23674 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.19891 HOMO: -6.51168 LUMO: 1.72520 factor:1 | 1 (-0.32128) | -1 | -1 |
| G: -6289.51193 HOMO: -6.61509 LUMO: -0.23674 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12553.93044 HOMO: -6.98516 LUMO: 1.92929 factor:1 | 1 (-0.05282) | -1 | -1 |
| G: -6289.51193 HOMO: -6.61509 LUMO: -0.23674 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.33929 HOMO: -6.92802 LUMO: 2.07895 factor:1 | 1 (-0.46167) | -1 | -1 |
| G: -6289.51193 HOMO: -6.61509 LUMO: -0.23674 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.55102 HOMO: -7.02326 LUMO: 1.86398 factor:1 | 1 (-0.67340) | -1 | -1 |
| G: -6289.51193 HOMO: -6.61509 LUMO: -0.23674 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.54346 HOMO: -6.82462 LUMO: 1.86670 factor:1 | 1 (-0.66584) | -1 | -1 |
| G: -6289.51193 HOMO: -6.61509 LUMO: -0.23674 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.52451 HOMO: -6.83278 LUMO: 1.71160 factor:1 | 1 (-1.64689) | -1 | -1 |
| G: -6289.51193 HOMO: -6.61509 LUMO: -0.23674 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.58799 HOMO: -6.62869 LUMO: 1.69527 factor:1 | 1 (-1.71037) | -1 | -1 |
| G: -6289.51193 HOMO: -6.61509 LUMO: -0.23674 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.34230 HOMO: -6.84094 LUMO: 1.27349 factor:1 | 1 (-1.46468) | -1 | -1 |
| G: -6289.51193 HOMO: -6.61509 LUMO: -0.23674 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.37732 HOMO: -7.07768 LUMO: 1.27621 factor:1 | 1 (-1.49970) | 1 | -1 |
| G: -6289.51193 HOMO: -6.61509 LUMO: -0.23674 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.20799 HOMO: -7.06135 LUMO: 1.55105 factor:1 | 1 (-1.33036) | 1 | -1 |
| G: -6289.51193 HOMO: -6.61509 LUMO: -0.23674 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.24102 HOMO: -6.94162 LUMO: 1.64629 factor:1 | 1 (-1.36340) | -1 | -1 |
| G: -6289.51193 HOMO: -6.61509 LUMO: -0.23674 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.19558 HOMO: -7.07224 LUMO: 1.65445 factor:1 | 1 (-1.31796) | 1 | -1 |
| G: -6289.51193 HOMO: -6.61509 LUMO: -0.23674 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.38140 HOMO: -6.68584 LUMO: 1.91296 factor:1 | 1 (-1.50378) | -1 | -1 |
| G: -6289.51193 HOMO: -6.61509 LUMO: -0.23674 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.28284 HOMO: -7.09129 LUMO: 1.73609 factor:1 | 1 (-1.40522) | 1 | -1 |
| G: -6289.51193 HOMO: -6.61509 LUMO: -0.23674 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.01748 HOMO: -7.01237 LUMO: 2.01092 factor:1 | 1 (-1.13986) | -1 | -1 |
| G: -6289.51193 HOMO: -6.61509 LUMO: -0.23674 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.35865 HOMO: -6.93618 LUMO: 1.63540 factor:1 | 1 (-1.48103) | -1 | -1 |
| G: -6289.51193 HOMO: -6.61509 LUMO: -0.23674 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.25729 HOMO: -6.98516 LUMO: 1.64629 factor:1 | 1 (-1.37967) | -1 | -1 |
| G: -6289.51193 HOMO: -6.61509 LUMO: -0.23674 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.27884 HOMO: -6.80285 LUMO: 1.95106 factor:1 | 1 (-1.40122) | -1 | -1 |
| G: -6289.51193 HOMO: -6.61509 LUMO: -0.23674 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.10858 HOMO: -6.76747 LUMO: 1.88303 factor:1 | 1 (-1.23096) | -1 | -1 |
| G: -6289.51193 HOMO: -6.61509 LUMO: -0.23674 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.32355 HOMO: -6.64230 LUMO: 1.90480 factor:1 | 1 (-1.44593) | -1 | -1 |
| G: -6289.51193 HOMO: -6.61509 LUMO: -0.23674 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.35972 HOMO: -6.93618 LUMO: 2.19324 factor:1 | 1 (-1.48210) | -1 | -1 |
| G: -6289.51193 HOMO: -6.61509 LUMO: -0.23674 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.51466 HOMO: -6.95523 LUMO: 1.80684 factor:1 | 1 (-1.63704) | -1 | -1 |
| G: -6289.51193 HOMO: -6.61509 LUMO: -0.23674 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.34935 HOMO: -6.66135 LUMO: 1.72792 factor:1 | 1 (-1.47173) | -1 | -1 |
| G: -6289.51193 HOMO: -6.61509 LUMO: -0.23674 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.16924 HOMO: -6.36202 LUMO: 1.89391 factor:1 | 1 (-1.29162) | -1 | -1 |
| G: -6289.51193 HOMO: -6.61509 LUMO: -0.23674 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.10091 HOMO: -7.03959 LUMO: 2.06262 factor:1 | 1 (-1.22329) | -1 | -1 |
| G: -6289.51193 HOMO: -6.61509 LUMO: -0.23674 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.39294 HOMO: -7.08584 LUMO: 2.01092 factor:1 | 1 (-1.51532) | 1 | -1 |
| G: -6289.51193 HOMO: -6.80285 LUMO: -0.55783 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.40271 HOMO: -6.96067 LUMO: 1.59731 factor:1 | 1 (-1.52509) | -1 | -1 |
| G: -6289.51193 HOMO: -6.80285 LUMO: -0.55783 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.43825 HOMO: -6.91169 LUMO: 1.37145 factor:1 | 1 (-1.56063) | -1 | -1 |
| G: -6289.51193 HOMO: -6.80285 LUMO: -0.55783 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.23220 HOMO: -6.94707 LUMO: 1.73064 factor:1 | 1 (-1.35458) | -1 | -1 |
| G: -6289.51193 HOMO: -6.80285 LUMO: -0.55783 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.40211 HOMO: -7.02326 LUMO: 1.41227 factor:1 | 1 (-1.52449) | -1 | -1 |
| G: -6289.51193 HOMO: -6.80285 LUMO: -0.55783 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.02986 HOMO: -6.72121 LUMO: 1.43132 factor:1 | 1 (-1.15224) | -1 | -1 |
| G: -6289.51193 HOMO: -6.80285 LUMO: -0.55783 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.99214 HOMO: -6.51168 LUMO: 1.72520 factor:1 | 1 (-1.11452) | -1 | -1 |
| G: -6289.51193 HOMO: -6.80285 LUMO: -0.55783 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.32070 HOMO: -6.98516 LUMO: 1.92929 factor:1 | 1 (-1.44307) | -1 | -1 |
| G: -6289.51193 HOMO: -6.80285 LUMO: -0.55783 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.17234 HOMO: -6.92802 LUMO: 2.07895 factor:1 | 1 (-1.29472) | -1 | -1 |
| G: -6289.51193 HOMO: -6.80285 LUMO: -0.55783 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.45336 HOMO: -7.02326 LUMO: 1.86398 factor:1 | 1 (-0.57574) | -1 | -1 |
| G: -6289.51193 HOMO: -6.80285 LUMO: -0.55783 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.56604 HOMO: -6.82462 LUMO: 1.86670 factor:1 | 1 (-0.68842) | -1 | -1 |
| G: -6289.51193 HOMO: -6.80285 LUMO: -0.55783 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.59407 HOMO: -6.83278 LUMO: 1.71160 factor:1 | 1 (-0.71645) | -1 | -1 |
| G: -6289.51193 HOMO: -6.80285 LUMO: -0.55783 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.70833 HOMO: -6.62869 LUMO: 1.69527 factor:1 | 1 (-0.83071) | -1 | -1 |
| G: -6289.51193 HOMO: -6.80285 LUMO: -0.55783 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.32947 HOMO: -6.84094 LUMO: 1.27349 factor:1 | 1 (-0.45185) | -1 | -1 |
| G: -6289.51193 HOMO: -6.80285 LUMO: -0.55783 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.38666 HOMO: -7.07768 LUMO: 1.27621 factor:1 | 1 (-0.50904) | 1 | -1 |
| G: -6289.51193 HOMO: -6.80285 LUMO: -0.55783 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.43706 HOMO: -7.06135 LUMO: 1.55105 factor:1 | 1 (-0.55944) | 1 | -1 |
| G: -6289.51193 HOMO: -6.80285 LUMO: -0.55783 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.62566 HOMO: -6.94162 LUMO: 1.64629 factor:1 | 1 (-0.74804) | -1 | -1 |
| G: -6289.51193 HOMO: -6.80285 LUMO: -0.55783 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.51948 HOMO: -7.07224 LUMO: 1.65445 factor:1 | 1 (-0.64186) | 1 | -1 |
| G: -6289.51193 HOMO: -6.80285 LUMO: -0.55783 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.48922 HOMO: -6.68584 LUMO: 1.91296 factor:1 | 1 (-0.61160) | -1 | -1 |
| G: -6289.51193 HOMO: -6.80285 LUMO: -0.55783 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.33834 HOMO: -7.09129 LUMO: 1.73609 factor:1 | 1 (-0.46072) | 1 | -1 |
| G: -6289.51193 HOMO: -6.80285 LUMO: -0.55783 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.45330 HOMO: -7.01237 LUMO: 2.01092 factor:1 | 1 (-1.57568) | -1 | -1 |
| G: -6289.51193 HOMO: -6.80285 LUMO: -0.55783 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.46927 HOMO: -6.93618 LUMO: 1.63540 factor:1 | 1 (-1.59165) | -1 | -1 |
| G: -6289.51193 HOMO: -6.80285 LUMO: -0.55783 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.21560 HOMO: -6.98516 LUMO: 1.64629 factor:1 | 1 (-1.33798) | -1 | -1 |
| G: -6289.51193 HOMO: -6.80285 LUMO: -0.55783 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.54524 HOMO: -6.80285 LUMO: 1.95106 factor:1 | 1 (-1.66762) | -1 | -1 |
| G: -6289.51193 HOMO: -6.80285 LUMO: -0.55783 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.30859 HOMO: -6.76747 LUMO: 1.88303 factor:1 | 1 (-1.43097) | -1 | -1 |
| G: -6289.51193 HOMO: -6.80285 LUMO: -0.55783 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.15718 HOMO: -6.64230 LUMO: 1.90480 factor:1 | 1 (-1.27956) | -1 | -1 |
| G: -6289.51193 HOMO: -6.80285 LUMO: -0.55783 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.97383 HOMO: -6.93618 LUMO: 2.19324 factor:1 | 1 (-1.09621) | -1 | -1 |
| G: -6289.51193 HOMO: -6.80285 LUMO: -0.55783 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.38042 HOMO: -6.95523 LUMO: 1.80684 factor:1 | 1 (-1.50280) | -1 | -1 |
| G: -6289.51193 HOMO: -6.80285 LUMO: -0.55783 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.17073 HOMO: -6.66135 LUMO: 1.72792 factor:1 | 1 (-1.29311) | -1 | -1 |
| G: -6289.51193 HOMO: -6.80285 LUMO: -0.55783 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.34355 HOMO: -6.36202 LUMO: 1.89391 factor:1 | 1 (-1.46593) | -1 | -1 |
| G: -6289.51193 HOMO: -6.80285 LUMO: -0.55783 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.29865 HOMO: -7.03959 LUMO: 2.06262 factor:1 | 1 (-1.42103) | -1 | -1 |
| G: -6289.51193 HOMO: -6.80285 LUMO: -0.55783 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.10551 HOMO: -7.08584 LUMO: 2.01092 factor:1 | 1 (-1.22789) | 1 | -1 |
| G: -6289.51193 HOMO: -7.16476 LUMO: 2.86264 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.00766 HOMO: -6.96067 LUMO: 1.59731 factor:1 | 1 (-1.13003) | -1 | -1 |
| G: -6289.51193 HOMO: -7.16476 LUMO: 2.86264 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.39501 HOMO: -6.91169 LUMO: 1.37145 factor:1 | 1 (-1.51739) | -1 | -1 |
| G: -6289.51193 HOMO: -7.16476 LUMO: 2.86264 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.25174 HOMO: -6.94707 LUMO: 1.73064 factor:1 | 1 (-1.37412) | -1 | -1 |
| G: -6289.51193 HOMO: -7.16476 LUMO: 2.86264 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.95043 HOMO: -7.02326 LUMO: 1.41227 factor:1 | 1 (-1.07281) | -1 | -1 |
| G: -6289.51193 HOMO: -7.16476 LUMO: 2.86264 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.90599 HOMO: -6.72121 LUMO: 1.43132 factor:1 | 1 (-1.02837) | -1 | -1 |
| G: -6289.51193 HOMO: -7.16476 LUMO: 2.86264 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.79331 HOMO: -6.51168 LUMO: 1.72520 factor:1 | 1 (-0.91569) | -1 | -1 |
| G: -6289.51193 HOMO: -7.16476 LUMO: 2.86264 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.46476 HOMO: -6.98516 LUMO: 1.92929 factor:1 | 1 (-0.58714) | -1 | -1 |
| G: -6289.51193 HOMO: -7.16476 LUMO: 2.86264 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.19547 HOMO: -6.92802 LUMO: 2.07895 factor:1 | 1 (-1.31785) | -1 | -1 |
| G: -6289.51193 HOMO: -7.16476 LUMO: 2.86264 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.06020 HOMO: -7.02326 LUMO: 1.86398 factor:1 | 1 (-1.18258) | -1 | -1 |
| G: -6289.51193 HOMO: -7.16476 LUMO: 2.86264 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.85639 HOMO: -6.82462 LUMO: 1.86670 factor:1 | 1 (-0.97877) | -1 | -1 |
| G: -6289.51193 HOMO: -7.16476 LUMO: 2.86264 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.24048 HOMO: -6.83278 LUMO: 1.71160 factor:1 | 1 (-1.36286) | -1 | -1 |
| G: -6289.51193 HOMO: -7.16476 LUMO: 2.86264 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.06317 HOMO: -6.62869 LUMO: 1.69527 factor:1 | 1 (-1.18555) | -1 | -1 |
| G: -6289.51193 HOMO: -7.16476 LUMO: 2.86264 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.20154 HOMO: -6.84094 LUMO: 1.27349 factor:1 | 1 (-1.32392) | -1 | -1 |
| G: -6289.51193 HOMO: -7.16476 LUMO: 2.86264 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.41819 HOMO: -7.07768 LUMO: 1.27621 factor:1 | 1 (-1.54057) | -1 | -1 |
| G: -6289.51193 HOMO: -7.16476 LUMO: 2.86264 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.97078 HOMO: -7.06135 LUMO: 1.55105 factor:1 | 1 (-1.09316) | -1 | -1 |
| G: -6289.51193 HOMO: -7.16476 LUMO: 2.86264 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.90708 HOMO: -6.94162 LUMO: 1.64629 factor:1 | 1 (-1.02946) | -1 | -1 |
| G: -6289.51193 HOMO: -7.16476 LUMO: 2.86264 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.99133 HOMO: -7.07224 LUMO: 1.65445 factor:1 | 1 (-1.11371) | -1 | -1 |
| G: -6289.51193 HOMO: -7.16476 LUMO: 2.86264 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.35686 HOMO: -6.68584 LUMO: 1.91296 factor:1 | 1 (-1.47924) | -1 | -1 |
| G: -6289.51193 HOMO: -7.16476 LUMO: 2.86264 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.15615 HOMO: -7.09129 LUMO: 1.73609 factor:1 | 1 (-1.27853) | -1 | -1 |
| G: -6289.51193 HOMO: -7.16476 LUMO: 2.86264 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.22790 HOMO: -7.01237 LUMO: 2.01092 factor:1 | 1 (-1.35028) | -1 | -1 |
| G: -6289.51193 HOMO: -7.16476 LUMO: 2.86264 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.13960 HOMO: -6.93618 LUMO: 1.63540 factor:1 | 1 (-1.26198) | -1 | -1 |
| G: -6289.51193 HOMO: -7.16476 LUMO: 2.86264 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.36355 HOMO: -6.98516 LUMO: 1.64629 factor:1 | 1 (-1.48593) | -1 | -1 |
| G: -6289.51193 HOMO: -7.16476 LUMO: 2.86264 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.86058 HOMO: -6.80285 LUMO: 1.95106 factor:1 | 1 (-0.98296) | -1 | -1 |
| G: -6289.51193 HOMO: -7.16476 LUMO: 2.86264 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.73361 HOMO: -6.76747 LUMO: 1.88303 factor:1 | 1 (-0.85599) | -1 | -1 |
| G: -6289.51193 HOMO: -7.16476 LUMO: 2.86264 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.83489 HOMO: -6.64230 LUMO: 1.90480 factor:1 | 1 (-0.95727) | -1 | -1 |
| G: -6289.51193 HOMO: -7.16476 LUMO: 2.86264 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.46999 HOMO: -6.93618 LUMO: 2.19324 factor:1 | 1 (-0.59236) | -1 | -1 |
| G: -6289.51193 HOMO: -7.16476 LUMO: 2.86264 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.11628 HOMO: -6.95523 LUMO: 1.80684 factor:1 | 1 (-1.23866) | -1 | -1 |
| G: -6289.51193 HOMO: -7.16476 LUMO: 2.86264 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.91271 HOMO: -6.66135 LUMO: 1.72792 factor:1 | 1 (-1.03509) | -1 | -1 |
| G: -6289.51193 HOMO: -7.16476 LUMO: 2.86264 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.90833 HOMO: -6.36202 LUMO: 1.89391 factor:1 | 1 (-1.03071) | -1 | -1 |
| G: -6289.51193 HOMO: -7.16476 LUMO: 2.86264 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.82675 HOMO: -7.03959 LUMO: 2.06262 factor:1 | 1 (-0.94913) | -1 | -1 |
| G: -6289.51193 HOMO: -7.16476 LUMO: 2.86264 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.64019 HOMO: -7.08584 LUMO: 2.01092 factor:1 | 1 (-0.76257) | -1 | -1 |
| G: -6289.51193 HOMO: -6.50352 LUMO: 2.10888 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.11182 HOMO: -6.96067 LUMO: 1.59731 factor:1 | 1 (-1.23420) | 1 | 1 |
| G: -6289.51193 HOMO: -6.50352 LUMO: 2.10888 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.80557 HOMO: -6.91169 LUMO: 1.37145 factor:1 | 1 (-1.92795) | -1 | -1 |
| G: -6289.51193 HOMO: -6.50352 LUMO: 2.10888 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12556.58268 HOMO: -6.94707 LUMO: 1.73064 factor:1 | 1 (-2.70506) | 1 | 1 |
| G: -6289.51193 HOMO: -6.50352 LUMO: 2.10888 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.45983 HOMO: -7.02326 LUMO: 1.41227 factor:1 | 1 (-1.58221) | -1 | -1 |
| G: -6289.51193 HOMO: -6.50352 LUMO: 2.10888 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.60160 HOMO: -6.72121 LUMO: 1.43132 factor:1 | 1 (-1.72398) | -1 | -1 |
| G: -6289.51193 HOMO: -6.50352 LUMO: 2.10888 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.80664 HOMO: -6.51168 LUMO: 1.72520 factor:1 | 1 (-1.92902) | 1 | 1 |
| G: -6289.51193 HOMO: -6.50352 LUMO: 2.10888 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.39713 HOMO: -6.98516 LUMO: 1.92929 factor:1 | 1 (-1.51951) | 1 | 1 |
| G: -6289.51193 HOMO: -6.50352 LUMO: 2.10888 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.89643 HOMO: -6.92802 LUMO: 2.07895 factor:1 | 1 (-2.01881) | 1 | 1 |
| G: -6289.51193 HOMO: -6.50352 LUMO: 2.10888 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12556.40423 HOMO: -7.02326 LUMO: 1.86398 factor:1 | 1 (-2.52660) | 1 | 1 |
| G: -6289.51193 HOMO: -6.50352 LUMO: 2.10888 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12556.12193 HOMO: -6.82462 LUMO: 1.86670 factor:1 | 1 (-2.24431) | 1 | 1 |
| G: -6289.51193 HOMO: -6.50352 LUMO: 2.10888 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12556.58015 HOMO: -6.83278 LUMO: 1.71160 factor:1 | 1 (-2.70253) | 1 | 1 |
| G: -6289.51193 HOMO: -6.50352 LUMO: 2.10888 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.42173 HOMO: -6.62869 LUMO: 1.69527 factor:1 | 1 (-1.54411) | 1 | 1 |
| G: -6289.51193 HOMO: -6.50352 LUMO: 2.10888 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.23816 HOMO: -6.84094 LUMO: 1.27349 factor:1 | 1 (-1.36054) | -1 | -1 |
| G: -6289.51193 HOMO: -6.50352 LUMO: 2.10888 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.05566 HOMO: -7.07768 LUMO: 1.27621 factor:1 | 1 (-1.17804) | -1 | -1 |
| G: -6289.51193 HOMO: -6.50352 LUMO: 2.10888 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12556.52153 HOMO: -7.06135 LUMO: 1.55105 factor:1 | 1 (-2.64391) | -1 | -1 |
| G: -6289.51193 HOMO: -6.50352 LUMO: 2.10888 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.73961 HOMO: -6.94162 LUMO: 1.64629 factor:1 | 1 (-1.86199) | 1 | 1 |
| G: -6289.51193 HOMO: -6.50352 LUMO: 2.10888 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12556.66714 HOMO: -7.07224 LUMO: 1.65445 factor:1 | 1 (-2.78952) | 1 | 1 |
| G: -6289.51193 HOMO: -6.50352 LUMO: 2.10888 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.36274 HOMO: -6.68584 LUMO: 1.91296 factor:1 | 1 (-1.48512) | 1 | 1 |
| G: -6289.51193 HOMO: -6.50352 LUMO: 2.10888 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12556.13257 HOMO: -7.09129 LUMO: 1.73609 factor:1 | 1 (-2.25495) | 1 | 1 |
| G: -6289.51193 HOMO: -6.50352 LUMO: 2.10888 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.88773 HOMO: -7.01237 LUMO: 2.01092 factor:1 | 1 (-2.01011) | 1 | 1 |
| G: -6289.51193 HOMO: -6.50352 LUMO: 2.10888 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.67365 HOMO: -6.93618 LUMO: 1.63540 factor:1 | 1 (-1.79603) | 1 | 1 |
| G: -6289.51193 HOMO: -6.50352 LUMO: 2.10888 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.52623 HOMO: -6.98516 LUMO: 1.64629 factor:1 | 1 (-0.64861) | 1 | 1 |
| G: -6289.51193 HOMO: -6.50352 LUMO: 2.10888 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.39515 HOMO: -6.80285 LUMO: 1.95106 factor:1 | 1 (-0.51753) | 1 | 1 |
| G: -6289.51193 HOMO: -6.50352 LUMO: 2.10888 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.93986 HOMO: -6.76747 LUMO: 1.88303 factor:1 | 1 (-2.06224) | 1 | 1 |
| G: -6289.51193 HOMO: -6.50352 LUMO: 2.10888 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.39808 HOMO: -6.64230 LUMO: 1.90480 factor:1 | 1 (-1.52046) | 1 | 1 |
| G: -6289.51193 HOMO: -6.50352 LUMO: 2.10888 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.79034 HOMO: -6.93618 LUMO: 2.19324 factor:1 | 1 (-1.91272) | 1 | 1 |
| G: -6289.51193 HOMO: -6.50352 LUMO: 2.10888 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.34219 HOMO: -6.95523 LUMO: 1.80684 factor:1 | 1 (-1.46457) | 1 | 1 |
| G: -6289.51193 HOMO: -6.50352 LUMO: 2.10888 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.28611 HOMO: -6.66135 LUMO: 1.72792 factor:1 | 1 (-1.40849) | 1 | 1 |
| G: -6289.51193 HOMO: -6.50352 LUMO: 2.10888 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.39599 HOMO: -6.36202 LUMO: 1.89391 factor:1 | 1 (-1.51837) | -1 | -1 |
| G: -6289.51193 HOMO: -6.50352 LUMO: 2.10888 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.31789 HOMO: -7.03959 LUMO: 2.06262 factor:1 | 1 (-1.44027) | 1 | 1 |
| G: -6289.51193 HOMO: -6.50352 LUMO: 2.10888 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.45928 HOMO: -7.08584 LUMO: 2.01092 factor:1 | 1 (-1.58166) | 1 | 1 |
| G: -6289.51193 HOMO: -6.59604 LUMO: 2.33746 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.24505 HOMO: -6.96067 LUMO: 1.59731 factor:1 | 1 (-1.36743) | 1 | 1 |
| G: -6289.51193 HOMO: -6.59604 LUMO: 2.33746 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.11258 HOMO: -6.91169 LUMO: 1.37145 factor:1 | 1 (-1.23496) | -1 | -1 |
| G: -6289.51193 HOMO: -6.59604 LUMO: 2.33746 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.18151 HOMO: -6.94707 LUMO: 1.73064 factor:1 | 1 (-1.30389) | 1 | 1 |
| G: -6289.51193 HOMO: -6.59604 LUMO: 2.33746 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.89111 HOMO: -7.02326 LUMO: 1.41227 factor:1 | 1 (-1.01349) | -1 | -1 |
| G: -6289.51193 HOMO: -6.59604 LUMO: 2.33746 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.63368 HOMO: -6.72121 LUMO: 1.43132 factor:1 | 1 (-1.75606) | -1 | -1 |
| G: -6289.51193 HOMO: -6.59604 LUMO: 2.33746 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.82449 HOMO: -6.51168 LUMO: 1.72520 factor:1 | 1 (-1.94687) | -1 | -1 |
| G: -6289.51193 HOMO: -6.59604 LUMO: 2.33746 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.62680 HOMO: -6.98516 LUMO: 1.92929 factor:1 | 1 (-1.74918) | 1 | 1 |
| G: -6289.51193 HOMO: -6.59604 LUMO: 2.33746 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.85341 HOMO: -6.92802 LUMO: 2.07895 factor:1 | 1 (-1.97579) | 1 | 1 |
| G: -6289.51193 HOMO: -6.59604 LUMO: 2.33746 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12556.43340 HOMO: -7.02326 LUMO: 1.86398 factor:1 | 1 (-2.55578) | 1 | 1 |
| G: -6289.51193 HOMO: -6.59604 LUMO: 2.33746 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.65975 HOMO: -6.82462 LUMO: 1.86670 factor:1 | 1 (-1.78213) | 1 | 1 |
| G: -6289.51193 HOMO: -6.59604 LUMO: 2.33746 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12556.13021 HOMO: -6.83278 LUMO: 1.71160 factor:1 | 1 (-2.25259) | 1 | 1 |
| G: -6289.51193 HOMO: -6.59604 LUMO: 2.33746 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12556.21704 HOMO: -6.62869 LUMO: 1.69527 factor:1 | 1 (-2.33942) | 1 | 1 |
| G: -6289.51193 HOMO: -6.59604 LUMO: 2.33746 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.49700 HOMO: -6.84094 LUMO: 1.27349 factor:1 | 1 (-1.61938) | -1 | -1 |
| G: -6289.51193 HOMO: -6.59604 LUMO: 2.33746 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12556.06212 HOMO: -7.07768 LUMO: 1.27621 factor:1 | 1 (-2.18450) | -1 | -1 |
| G: -6289.51193 HOMO: -6.59604 LUMO: 2.33746 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.34369 HOMO: -7.06135 LUMO: 1.55105 factor:1 | 1 (-1.46607) | -1 | -1 |
| G: -6289.51193 HOMO: -6.59604 LUMO: 2.33746 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.41808 HOMO: -6.94162 LUMO: 1.64629 factor:1 | 1 (-1.54046) | 1 | 1 |
| G: -6289.51193 HOMO: -6.59604 LUMO: 2.33746 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.62152 HOMO: -7.07224 LUMO: 1.65445 factor:1 | 1 (-1.74390) | 1 | 1 |
| G: -6289.51193 HOMO: -6.59604 LUMO: 2.33746 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.46562 HOMO: -6.68584 LUMO: 1.91296 factor:1 | 1 (-1.58800) | 1 | 1 |
| G: -6289.51193 HOMO: -6.59604 LUMO: 2.33746 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.23713 HOMO: -7.09129 LUMO: 1.73609 factor:1 | 1 (-1.35951) | 1 | 1 |
| G: -6289.51193 HOMO: -6.59604 LUMO: 2.33746 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.25264 HOMO: -7.01237 LUMO: 2.01092 factor:1 | 1 (-1.37502) | 1 | 1 |
| G: -6289.51193 HOMO: -6.59604 LUMO: 2.33746 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.60455 HOMO: -6.93618 LUMO: 1.63540 factor:1 | 1 (-0.72692) | 1 | 1 |
| G: -6289.51193 HOMO: -6.59604 LUMO: 2.33746 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.38381 HOMO: -6.98516 LUMO: 1.64629 factor:1 | 1 (-0.50619) | 1 | 1 |
| G: -6289.51193 HOMO: -6.59604 LUMO: 2.33746 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.30209 HOMO: -6.80285 LUMO: 1.95106 factor:1 | 1 (-0.42447) | 1 | 1 |
| G: -6289.51193 HOMO: -6.59604 LUMO: 2.33746 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.56188 HOMO: -6.76747 LUMO: 1.88303 factor:1 | 1 (-0.68426) | 1 | 1 |
| G: -6289.51193 HOMO: -6.59604 LUMO: 2.33746 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.51208 HOMO: -6.64230 LUMO: 1.90480 factor:1 | 1 (-0.63446) | 1 | 1 |
| G: -6289.51193 HOMO: -6.59604 LUMO: 2.33746 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.11390 HOMO: -6.93618 LUMO: 2.19324 factor:1 | 1 (-0.23628) | 1 | 1 |
| G: -6289.51193 HOMO: -6.59604 LUMO: 2.33746 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.38879 HOMO: -6.95523 LUMO: 1.80684 factor:1 | 1 (-0.51117) | 1 | 1 |
| G: -6289.51193 HOMO: -6.59604 LUMO: 2.33746 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.31853 HOMO: -6.66135 LUMO: 1.72792 factor:1 | 1 (-0.44091) | 1 | 1 |
| G: -6289.51193 HOMO: -6.59604 LUMO: 2.33746 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.34990 HOMO: -6.36202 LUMO: 1.89391 factor:1 | 1 (-0.47228) | -1 | -1 |
| G: -6289.51193 HOMO: -6.59604 LUMO: 2.33746 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.18759 HOMO: -7.03959 LUMO: 2.06262 factor:1 | 1 (-0.30996) | 1 | 1 |
| G: -6289.51193 HOMO: -6.59604 LUMO: 2.33746 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.54659 HOMO: -7.08584 LUMO: 2.01092 factor:1 | 1 (-0.66896) | 1 | 1 |
| G: -6289.51193 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.32462 HOMO: -7.06135 LUMO: 0.75376 factor:1 | 1 (-0.44700) | 1 | -1 |
| G: -6289.51193 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.71787 HOMO: -5.10213 LUMO: 0.77825 factor:1 | 1 (-1.84025) | -1 | -1 |
| G: -6289.51193 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12556.50834 HOMO: -5.84228 LUMO: 0.50341 factor:1 | 1 (-2.63072) | -1 | -1 |
| G: -6289.51193 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12556.25900 HOMO: -5.39874 LUMO: 0.68028 factor:1 | 1 (-2.38138) | -1 | -1 |
| G: -6289.51193 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.60573 HOMO: -5.16744 LUMO: 1.14832 factor:1 | 1 (-1.72811) | -1 | -1 |
| G: -6289.51193 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.16707 HOMO: -5.80963 LUMO: 0.35647 factor:1 | 1 (-0.28945) | -1 | -1 |
| G: -6289.51193 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.39722 HOMO: -5.02322 LUMO: 1.07213 factor:1 | 1 (-0.51960) | -1 | -1 |
| G: -6289.51193 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.86778 HOMO: -5.80963 LUMO: 0.56328 factor:1 | 1 (-1.99016) | -1 | -1 |
| G: -6289.51193 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.19786 HOMO: -5.45316 LUMO: 0.78369 factor:1 | 1 (-1.32024) | -1 | -1 |
| G: -6289.51193 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12556.00384 HOMO: -5.25452 LUMO: 0.82178 factor:1 | 1 (-2.12622) | -1 | -1 |
| G: -6289.51193 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.90718 HOMO: -5.21370 LUMO: 1.03947 factor:1 | 1 (-2.02956) | -1 | -1 |
| G: -6289.51193 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.69028 HOMO: -6.04365 LUMO: 0.31837 factor:1 | 1 (-1.81266) | -1 | -1 |
| G: -6289.51193 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.97155 HOMO: -5.86405 LUMO: 0.55511 factor:1 | 1 (-1.09392) | -1 | -1 |
| G: -6289.51193 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.27920 HOMO: -5.64908 LUMO: 0.71022 factor:1 | 1 (-1.40158) | -1 | -1 |
| G: -6289.51193 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.40753 HOMO: -5.94297 LUMO: 0.68301 factor:1 | 1 (-1.52991) | -1 | -1 |
| G: -6289.51193 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.37204 HOMO: -6.01916 LUMO: 0.56328 factor:1 | 1 (-1.49442) | -1 | -1 |
| G: -6289.51193 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.35400 HOMO: -6.05181 LUMO: 0.35103 factor:1 | 1 (-1.47638) | -1 | -1 |
| G: -6289.51193 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.26965 HOMO: -6.08447 LUMO: 0.48436 factor:1 | 1 (-1.39203) | -1 | -1 |
| G: -6289.51193 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.56494 HOMO: -5.86950 LUMO: 0.36735 factor:1 | 1 (-1.68732) | -1 | -1 |
| G: -6289.51193 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.58816 HOMO: -5.33615 LUMO: 0.65852 factor:1 | 1 (-1.71053) | -1 | -1 |
| G: -6289.51193 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.36513 HOMO: -5.36064 LUMO: 0.86804 factor:1 | 1 (-1.48751) | -1 | -1 |
| G: -6289.51193 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.40862 HOMO: -5.74160 LUMO: 0.64491 factor:1 | 1 (-1.53099) | -1 | -1 |
| G: -6289.51193 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.10551 HOMO: -5.23003 LUMO: 0.66124 factor:1 | 1 (-1.22789) | -1 | -1 |
| G: -6289.51193 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.22761 HOMO: -5.77698 LUMO: 0.84083 factor:1 | 1 (-0.34999) | -1 | -1 |
| G: -6289.51193 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.08201 HOMO: -5.60555 LUMO: 0.84355 factor:1 | 1 (-0.20438) | -1 | -1 |
| G: -6289.51193 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.09991 HOMO: -7.11578 LUMO: -1.62452 factor:1 | 1 (-0.22229) | -1 | -1 |
| G: -6289.51193 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12553.83993 HOMO: -7.23279 LUMO: -1.63813 factor:1 | -1 (0.03769) | -1 | -1 |
| G: -6289.51193 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.28459 HOMO: -6.68312 LUMO: -0.88709 factor:1 | 1 (-0.40697) | -1 | -1 |
| G: -6289.51193 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.99962 HOMO: -6.99333 LUMO: -0.88709 factor:1 | 1 (-2.12200) | -1 | -1 |
| G: -6289.51193 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.73978 HOMO: -7.40694 LUMO: 0.11973 factor:1 | 1 (-1.86216) | 1 | 1 |
| G: -6289.51193 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12556.05709 HOMO: -6.74026 LUMO: -0.72927 factor:1 | 1 (-2.17947) | -1 | -1 |
| G: -6289.51193 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.32848 HOMO: -6.67223 LUMO: -0.70750 factor:1 | 1 (-1.45086) | -1 | -1 |
| G: -6289.51193 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.05522 HOMO: -7.06952 LUMO: -1.40139 factor:1 | 1 (-1.17760) | -1 | -1 |
| G: -6289.51193 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.89976 HOMO: -7.21374 LUMO: -1.13199 factor:1 | 1 (-1.02214) | -1 | -1 |
| G: -6289.51193 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.09280 HOMO: -6.54706 LUMO: -1.34424 factor:1 | 1 (-1.21518) | -1 | -1 |
| G: -6289.51193 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.24516 HOMO: -7.51851 LUMO: -1.05852 factor:1 | 1 (-1.36754) | -1 | -1 |
| G: -6289.51193 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.22695 HOMO: -7.07224 LUMO: -1.89391 factor:1 | 1 (-1.34933) | -1 | -1 |
| G: -6289.51193 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.92885 HOMO: -6.65863 LUMO: -0.46804 factor:1 | 1 (-1.05123) | -1 | -1 |
| G: -6289.51193 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.04507 HOMO: -7.24367 LUMO: 0.29388 factor:1 | 1 (-1.16745) | 1 | 1 |
| G: -6289.51193 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.79405 HOMO: -7.02326 LUMO: -0.87893 factor:1 | 1 (-0.91643) | -1 | -1 |
| G: -6289.51193 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.23476 HOMO: -6.88176 LUMO: 0.71566 factor:1 | 1 (-1.35714) | -1 | -1 |
| G: -6289.51193 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.38944 HOMO: -6.46543 LUMO: 1.01498 factor:1 | 1 (-0.51182) | -1 | -1 |
| G: -6289.51193 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.58509 HOMO: -6.30760 LUMO: 0.17687 factor:1 | 1 (-0.70747) | -1 | -1 |
| G: -6289.51193 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.52014 HOMO: -6.73210 LUMO: -1.06941 factor:1 | 1 (-0.64252) | -1 | -1 |
| G: -6289.51193 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.48637 HOMO: -6.83550 LUMO: -0.75920 factor:1 | 1 (-0.60875) | -1 | -1 |
| G: -6289.51193 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.19240 HOMO: -6.94707 LUMO: 0.42178 factor:1 | 1 (-0.31478) | -1 | -1 |
| G: -6289.51193 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.33186 HOMO: -6.77019 LUMO: -0.38096 factor:1 | 1 (-0.45424) | -1 | -1 |
| G: -6289.51193 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.55497 HOMO: -7.34163 LUMO: 0.35103 factor:1 | 1 (-0.67735) | 1 | 1 |
| G: -6289.51193 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.78414 HOMO: -6.87632 LUMO: -0.87349 factor:1 | 1 (-0.90652) | -1 | -1 |
| G: -6289.51193 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.75535 HOMO: -7.06952 LUMO: -1.47214 factor:1 | 1 (-0.87773) | -1 | -1 |
| G: -6289.51193 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.48022 HOMO: -6.58788 LUMO: -0.37824 factor:1 | 1 (-0.60260) | -1 | -1 |
| G: -6289.51193 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.55739 HOMO: -6.92802 LUMO: -1.24900 factor:1 | 1 (-0.67977) | -1 | -1 |
| G: -6289.51193 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.23123 HOMO: -7.01237 LUMO: -1.31975 factor:1 | 1 (-0.35361) | -1 | -1 |
| G: -6289.51193 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.33513 HOMO: -6.74842 LUMO: 0.45987 factor:1 | 1 (-0.45751) | -1 | -1 |
| G: -6289.51193 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.20522 HOMO: -6.53890 LUMO: 0.94424 factor:1 | 1 (-0.32760) | -1 | -1 |
| G: -6289.51193 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.04503 HOMO: -6.52257 LUMO: -0.66940 factor:1 | 1 (-0.16740) | -1 | -1 |
| G: -6289.51193 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.33567 HOMO: -6.56883 LUMO: -1.48302 factor:1 | 1 (-0.45805) | -1 | -1 |
| G: -6289.51193 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.57415 HOMO: -7.21646 LUMO: 0.13061 factor:1 | 1 (-0.69653) | 1 | 1 |
| G: -6289.51193 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.62776 HOMO: -6.62597 LUMO: -0.64763 factor:1 | 1 (-0.75014) | -1 | -1 |
| G: -6289.51193 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.35330 HOMO: -7.38789 LUMO: 0.31021 factor:1 | 1 (-0.47568) | 1 | 1 |
| G: -6289.51193 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.57284 HOMO: -6.74570 LUMO: -0.70750 factor:1 | 1 (-0.69522) | -1 | -1 |
| G: -6289.51193 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.47042 HOMO: -6.95251 LUMO: -1.25989 factor:1 | 1 (-0.59280) | -1 | -1 |
| G: -6289.51193 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.67026 HOMO: -7.13483 LUMO: -0.76736 factor:1 | 1 (-0.79264) | -1 | -1 |
| G: -6289.51193 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.17052 HOMO: -6.93618 LUMO: -1.24628 factor:1 | 1 (-1.29289) | -1 | -1 |
| G: -6289.51193 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.33591 HOMO: -7.03686 LUMO: 0.26395 factor:1 | 1 (-1.45829) | -1 | -1 |
| G: -6289.51193 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.04330 HOMO: -6.52257 LUMO: -0.84355 factor:1 | 1 (-1.16568) | -1 | -1 |
| G: -6289.51193 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.11054 HOMO: -6.83278 LUMO: -0.49525 factor:1 | 1 (-1.23292) | -1 | -1 |
| G: -6289.51193 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.02442 HOMO: -7.18381 LUMO: -1.64629 factor:1 | 1 (-1.14680) | -1 | -1 |
| G: -6289.51193 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.08181 HOMO: -6.74842 LUMO: -0.81090 factor:1 | 1 (-1.20419) | -1 | -1 |
| G: -6289.51193 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.56985 HOMO: -7.09401 LUMO: -0.92519 factor:1 | 1 (-0.69223) | -1 | -1 |
| G: -6289.51193 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.31379 HOMO: -7.20285 LUMO: -0.81634 factor:1 | 1 (-0.43617) | -1 | -1 |
| G: -6289.51193 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.13295 HOMO: -6.72665 LUMO: 0.77008 factor:1 | 1 (-0.25532) | -1 | -1 |
| G: -6289.51193 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12553.95498 HOMO: -6.80829 LUMO: 0.86532 factor:1 | 1 (-0.07736) | -1 | -1 |
| G: -6289.51193 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.25401 HOMO: -6.20964 LUMO: 0.99866 factor:1 | 1 (-0.37639) | -1 | -1 |
| G: -6289.51193 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.38432 HOMO: -6.52801 LUMO: 1.07757 factor:1 | 1 (-0.50670) | -1 | -1 |
| G: -6289.51193 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.34198 HOMO: -6.74298 LUMO: -0.67756 factor:1 | 1 (-0.46436) | -1 | -1 |
| G: -6289.51193 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.29774 HOMO: -7.43959 LUMO: 0.03265 factor:1 | 1 (-0.42012) | 1 | 1 |
| G: -6289.51193 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.05771 HOMO: -6.46815 LUMO: -0.29933 factor:1 | 1 (-0.18008) | -1 | -1 |
| G: -6289.51193 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.25414 HOMO: -6.70489 LUMO: -0.97145 factor:1 | 1 (-0.37652) | -1 | -1 |
| G: -6289.51193 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.15757 HOMO: -6.30216 LUMO: -1.39322 factor:1 | 1 (-0.27995) | -1 | -1 |
| G: -6289.51193 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12553.84864 HOMO: -7.01782 LUMO: -1.07485 factor:1 | -1 (0.02898) | -1 | -1 |
| G: -6289.51193 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.50375 HOMO: -6.93074 LUMO: 0.25851 factor:1 | 1 (-0.62613) | -1 | -1 |
| G: -6289.51193 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.16968 HOMO: -7.07224 LUMO: 0.09524 factor:1 | 1 (-0.29206) | 1 | 1 |
| G: -6289.51193 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.49959 HOMO: -6.62325 LUMO: -0.45443 factor:1 | 1 (-0.62197) | -1 | -1 |
| G: -6289.51193 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.33608 HOMO: -7.09945 LUMO: -1.20274 factor:1 | 1 (-0.45846) | -1 | -1 |
| G: -6289.51193 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.13009 HOMO: -6.56067 LUMO: -1.39322 factor:1 | 1 (-0.25247) | -1 | -1 |
| G: -6289.51193 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12553.82959 HOMO: -6.75387 LUMO: -0.72654 factor:1 | -1 (0.04803) | -1 | -1 |
| G: -6289.51193 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.32528 HOMO: -6.28583 LUMO: -2.35651 factor:1 | 1 (-0.44765) | -1 | -1 |
| G: -6289.51193 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.51233 HOMO: -6.55522 LUMO: -1.33608 factor:1 | 1 (-0.63471) | -1 | -1 |
| G: -6289.51193 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.45235 HOMO: -7.19741 LUMO: -0.93607 factor:1 | 1 (-0.57473) | -1 | -1 |
| G: -6289.51193 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.26253 HOMO: -6.39740 LUMO: -1.14832 factor:1 | 1 (-0.38491) | -1 | -1 |
| G: -6289.51193 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.26508 HOMO: -7.11850 LUMO: -0.97417 factor:1 | 1 (-0.38746) | -1 | -1 |
| G: -6289.51193 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12553.90959 HOMO: -6.57699 LUMO: -1.14016 factor:1 | 1 (-0.03197) | -1 | -1 |
| G: -6289.51193 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.08103 HOMO: -6.57699 LUMO: -1.31975 factor:1 | 1 (-0.20341) | -1 | -1 |
| G: -6289.51193 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.10432 HOMO: -6.69128 LUMO: -0.76736 factor:1 | 1 (-0.22670) | -1 | -1 |
| G: -6289.51193 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12553.83237 HOMO: -7.25728 LUMO: 0.29660 factor:1 | -1 (0.04525) | 1 | 1 |
| G: -6289.51193 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.36974 HOMO: -6.37019 LUMO: -0.95240 factor:1 | 1 (-0.49212) | -1 | -1 |
| G: -6289.51193 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.66830 HOMO: -6.48447 LUMO: -0.55511 factor:1 | 1 (-0.79068) | -1 | -1 |
| G: -6289.51193 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.43494 HOMO: -6.37291 LUMO: -0.78641 factor:1 | 1 (-0.55732) | -1 | -1 |
| G: -6289.51193 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.58071 HOMO: -6.65863 LUMO: -0.69933 factor:1 | 1 (-0.70309) | -1 | -1 |
| G: -6289.51193 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.66626 HOMO: -6.44638 LUMO: -0.16055 factor:1 | 1 (-0.78864) | -1 | -1 |
| G: -6289.51193 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.72863 HOMO: -6.41917 LUMO: -0.20136 factor:1 | 1 (-0.85101) | -1 | -1 |
| G: -6289.51193 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.43926 HOMO: -7.33347 LUMO: 0.12789 factor:1 | 1 (-0.56164) | 1 | 1 |
| G: -6289.51193 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.39200 HOMO: -6.70489 LUMO: -0.52518 factor:1 | 1 (-0.51438) | -1 | -1 |
| G: -6289.51193 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.64134 HOMO: -7.25183 LUMO: 0.32109 factor:1 | 1 (-0.76371) | 1 | 1 |
| G: -6289.51193 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.34030 HOMO: -7.29265 LUMO: 0.28028 factor:1 | 1 (-0.46268) | 1 | 1 |
| G: -6289.51193 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.58479 HOMO: -6.57155 LUMO: -0.51702 factor:1 | 1 (-0.70717) | -1 | -1 |
| G: -6289.51193 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.62939 HOMO: -7.08040 LUMO: 0.39729 factor:1 | 1 (-0.75177) | 1 | 1 |
| G: -6289.51193 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.41983 HOMO: -6.24501 LUMO: -0.44627 factor:1 | 1 (-0.54221) | -1 | -1 |
| G: -6289.51193 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.28323 HOMO: -6.73754 LUMO: -0.45443 factor:1 | 1 (-0.40561) | -1 | -1 |
| G: -6289.51193 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.36514 HOMO: -6.24501 LUMO: 0.38096 factor:1 | 1 (-0.48752) | -1 | -1 |
| G: -6289.51193 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.48258 HOMO: -6.86815 LUMO: -0.91974 factor:1 | 1 (-0.60496) | -1 | -1 |
| G: -6289.51193 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.52792 HOMO: -7.40150 LUMO: 0.36191 factor:1 | 1 (-0.65030) | 1 | 1 |
| G: -6289.51193 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.32729 HOMO: -6.44094 LUMO: -0.64219 factor:1 | 1 (-0.44967) | -1 | -1 |
| G: -6289.51193 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.14002 HOMO: -6.69944 LUMO: -0.80001 factor:1 | 1 (-0.26240) | -1 | -1 |
| G: -6289.51193 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12553.86426 HOMO: -6.61509 LUMO: -0.70750 factor:1 | -1 (0.01336) | -1 | -1 |
| G: -6289.51193 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.39219 HOMO: -7.52123 LUMO: 0.06803 factor:1 | 1 (-0.51457) | 1 | 1 |
| G: -6289.51193 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.37025 HOMO: -7.34163 LUMO: 0.30477 factor:1 | 1 (-1.49263) | 1 | 1 |
| G: -6289.51193 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.39411 HOMO: -6.68584 LUMO: -0.78641 factor:1 | 1 (-1.51649) | -1 | -1 |
| G: -6289.51193 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.37863 HOMO: -6.53890 LUMO: -0.50885 factor:1 | 1 (-1.50101) | -1 | -1 |
| G: -6289.51193 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.95620 HOMO: -6.75659 LUMO: -0.68845 factor:1 | 1 (-1.07858) | -1 | -1 |
| G: -6289.51193 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.18173 HOMO: -7.08857 LUMO: 0.43266 factor:1 | 1 (-1.30411) | 1 | 1 |
| G: -6289.51193 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.09231 HOMO: -6.28583 LUMO: -0.46804 factor:1 | 1 (-1.21469) | -1 | -1 |
| G: -6289.51193 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.16377 HOMO: -6.50080 LUMO: -0.24762 factor:1 | 1 (-1.28615) | -1 | -1 |
| G: -6289.51193 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.60196 HOMO: -6.45454 LUMO: -0.58504 factor:1 | 1 (-0.72434) | -1 | -1 |
| G: -6289.51193 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.35189 HOMO: -7.20558 LUMO: 0.20953 factor:1 | 1 (-0.47427) | 1 | 1 |
| G: -6289.51193 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.38612 HOMO: -6.35930 LUMO: -0.20681 factor:1 | 1 (-0.50850) | -1 | -1 |
| G: -6289.51193 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.20595 HOMO: -6.36202 LUMO: -0.14422 factor:1 | 1 (-0.32833) | -1 | -1 |
| G: -6289.51193 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.16097 HOMO: -6.20692 LUMO: 1.97827 factor:1 | 1 (-0.28335) | -1 | -1 |
| G: -6289.51193 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.10116 HOMO: -6.48719 LUMO: 1.74153 factor:1 | 1 (-0.22354) | -1 | -1 |
| G: -6289.51193 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12553.93531 HOMO: -6.84638 LUMO: 1.88575 factor:1 | 1 (-0.05769) | -1 | -1 |
| G: -6289.51193 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.35110 HOMO: -5.90759 LUMO: 2.00820 factor:1 | 1 (-0.47348) | -1 | -1 |
| G: -6289.51193 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.32440 HOMO: -6.56339 LUMO: 1.99732 factor:1 | 1 (-0.44678) | -1 | -1 |
| G: -6289.51193 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.20744 HOMO: -6.20692 LUMO: 1.75241 factor:1 | 1 (-1.32982) | -1 | -1 |
| G: -6289.51193 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.05487 HOMO: -6.16882 LUMO: 1.94017 factor:1 | 1 (-1.17725) | -1 | -1 |
| G: -6289.51193 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.49463 HOMO: -6.80829 LUMO: 1.78507 factor:1 | 1 (-1.61701) | -1 | -1 |
| G: -6289.51193 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.84360 HOMO: -6.58243 LUMO: 1.78235 factor:1 | 1 (-0.96598) | -1 | -1 |
| G: -6289.51193 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.88308 HOMO: -5.85045 LUMO: 1.82316 factor:1 | 1 (-1.00546) | -1 | -1 |
| G: -6289.51193 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.97971 HOMO: -5.93752 LUMO: 1.56465 factor:1 | 1 (-1.10209) | -1 | -1 |
| G: -6289.51193 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.00752 HOMO: -6.59604 LUMO: -0.53334 factor:1 | 1 (-1.12990) | -1 | -1 |
| G: -6289.51193 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.14012 HOMO: -7.06135 LUMO: 0.29660 factor:1 | 1 (-1.26250) | 1 | 1 |
| G: -6289.51193 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.13383 HOMO: -6.50352 LUMO: 1.61908 factor:1 | 1 (-1.25621) | -1 | -1 |
| G: -6289.51193 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.04123 HOMO: -6.68040 LUMO: -0.60681 factor:1 | 1 (-1.16361) | -1 | -1 |
| G: -6289.51193 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.98518 HOMO: -6.93618 LUMO: -1.09662 factor:1 | 1 (-1.10756) | -1 | -1 |
| G: -6289.51193 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.75995 HOMO: -6.72121 LUMO: -1.14016 factor:1 | 1 (-0.88233) | -1 | -1 |
| G: -6289.51193 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.87633 HOMO: -7.12394 LUMO: -1.24900 factor:1 | 1 (-0.99871) | -1 | -1 |
| G: -6289.51193 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.93152 HOMO: -6.71305 LUMO: -0.71566 factor:1 | 1 (-1.05390) | -1 | -1 |
| G: -6289.51193 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.22355 HOMO: -7.09401 LUMO: -0.86532 factor:1 | 1 (-1.34593) | -1 | -1 |
| G: -6289.51193 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.00306 HOMO: -7.08584 LUMO: -0.92519 factor:1 | 1 (-1.12544) | -1 | -1 |
| G: -6289.51193 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.05166 HOMO: -7.05591 LUMO: 0.11973 factor:1 | 1 (-1.17404) | -1 | -1 |
| G: -6289.51193 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.29898 HOMO: -7.14843 LUMO: -1.58370 factor:1 | 1 (-1.42136) | -1 | -1 |
| G: -6289.51193 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12556.42110 HOMO: -7.36884 LUMO: -1.97010 factor:1 | 1 (-2.54348) | -1 | -1 |
| G: -6289.51193 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.79624 HOMO: -6.81373 LUMO: -1.72248 factor:1 | 1 (-1.91862) | -1 | -1 |
| G: -6289.51193 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12556.57737 HOMO: -6.87360 LUMO: -1.03947 factor:1 | 1 (-2.69975) | -1 | -1 |
| G: -6289.51193 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.59235 HOMO: -7.02870 LUMO: -0.87349 factor:1 | 1 (-1.71473) | -1 | -1 |
| G: -6289.51193 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.61006 HOMO: -7.16476 LUMO: -1.18097 factor:1 | 1 (-1.73244) | -1 | -1 |
| G: -6289.51193 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12556.43644 HOMO: -7.51851 LUMO: 0.07891 factor:1 | 1 (-2.55882) | 1 | 1 |
| G: -6289.51193 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12556.39827 HOMO: -7.04231 LUMO: -0.83539 factor:1 | 1 (-2.52065) | -1 | -1 |
| G: -6289.51193 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12556.01633 HOMO: -6.83278 LUMO: -0.60137 factor:1 | 1 (-2.13871) | -1 | -1 |
| G: -6289.51193 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12556.39759 HOMO: -6.89809 LUMO: -1.19186 factor:1 | 1 (-2.51996) | -1 | -1 |
| G: -6289.51193 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12556.20077 HOMO: -7.16476 LUMO: -0.79185 factor:1 | 1 (-2.32314) | -1 | -1 |
| G: -6289.51193 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.41242 HOMO: -6.97156 LUMO: -1.25444 factor:1 | 1 (-1.53480) | -1 | -1 |
| G: -6289.51193 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.98346 HOMO: -6.84366 LUMO: -0.88437 factor:1 | 1 (-1.10584) | -1 | -1 |
| G: -6289.51193 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12556.16076 HOMO: -6.91986 LUMO: -1.12655 factor:1 | 1 (-2.28314) | -1 | -1 |
| G: -6289.51193 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.26867 HOMO: -6.49536 LUMO: -0.29660 factor:1 | 1 (-1.39105) | -1 | -1 |
| G: -6289.51193 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.42004 HOMO: -6.74842 LUMO: 0.42450 factor:1 | 1 (-1.54242) | -1 | -1 |
| G: -6289.51193 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.04847 HOMO: -7.34435 LUMO: 0.32109 factor:1 | 1 (-1.17085) | 1 | 1 |
| G: -6289.51193 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.61213 HOMO: -7.16476 LUMO: 0.28572 factor:1 | 1 (-1.73451) | 1 | 1 |
| G: -6289.51193 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.33278 HOMO: -6.74298 LUMO: -0.43538 factor:1 | 1 (-1.45516) | -1 | -1 |
| G: -6289.51193 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.43545 HOMO: -7.19469 LUMO: -1.61091 factor:1 | 1 (-1.55782) | -1 | -1 |
| G: -6289.51193 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.48143 HOMO: -7.35252 LUMO: -1.78235 factor:1 | 1 (-1.60381) | -1 | -1 |
| G: -6289.51193 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.35574 HOMO: -7.25456 LUMO: -1.66806 factor:1 | 1 (-1.47812) | -1 | -1 |
| G: -6289.51193 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.79926 HOMO: -7.54844 LUMO: -1.07213 factor:1 | 1 (-1.92164) | -1 | -1 |
| G: -6289.51193 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.60688 HOMO: -7.21918 LUMO: -1.55377 factor:1 | 1 (-1.72926) | -1 | -1 |
| G: -6289.51193 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.64473 HOMO: -7.01782 LUMO: -1.60547 factor:1 | 1 (-1.76711) | -1 | -1 |
| G: -6289.51193 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.61575 HOMO: -7.21646 LUMO: -1.53472 factor:1 | 1 (-1.73813) | -1 | -1 |
| G: -6289.51193 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.23956 HOMO: -6.73754 LUMO: -1.37417 factor:1 | 1 (-0.36194) | -1 | -1 |
| G: -6289.51193 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.40013 HOMO: -6.78924 LUMO: 0.66396 factor:1 | 1 (-0.52251) | -1 | -1 |
| G: -6289.51193 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.24974 HOMO: -6.82734 LUMO: 0.61226 factor:1 | 1 (-0.37212) | -1 | -1 |
| G: -6289.51193 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.44525 HOMO: -6.74026 LUMO: 0.65579 factor:1 | 1 (-0.56763) | -1 | -1 |
| G: -6289.51193 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.32143 HOMO: -7.10489 LUMO: -1.30887 factor:1 | 1 (-1.44381) | -1 | -1 |
| G: -6289.51193 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12556.03823 HOMO: -7.05047 LUMO: 0.42722 factor:1 | 1 (-2.16061) | -1 | -1 |
| G: -6289.51193 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.97173 HOMO: -6.61237 LUMO: 1.30887 factor:1 | 1 (-2.09411) | -1 | -1 |
| G: -6289.51193 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.33612 HOMO: -7.05863 LUMO: 0.59049 factor:1 | 1 (-1.45850) | -1 | -1 |
| G: -6289.51193 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.81398 HOMO: -6.26406 LUMO: 0.78641 factor:1 | 1 (-1.93636) | -1 | -1 |
| G: -6289.51193 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.16886 HOMO: -6.70489 LUMO: 0.67756 factor:1 | 1 (-1.29123) | -1 | -1 |
| G: -6289.51193 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.36393 HOMO: -6.78652 LUMO: -0.94968 factor:1 | 1 (-1.48631) | -1 | -1 |
| G: -6289.51193 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.28576 HOMO: -6.36202 LUMO: -0.94424 factor:1 | 1 (-1.40813) | -1 | -1 |
| G: -6289.51193 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.25599 HOMO: -6.81645 LUMO: -1.09934 factor:1 | 1 (-1.37837) | -1 | -1 |
| G: -6289.51193 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.29974 HOMO: -7.07224 LUMO: 0.85988 factor:1 | 1 (-1.42212) | 1 | 1 |
| G: -6289.51193 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.93582 HOMO: -7.02326 LUMO: 1.10206 factor:1 | 1 (-1.05820) | -1 | -1 |
| G: -6289.51193 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.07421 HOMO: -6.71305 LUMO: 0.84627 factor:1 | 1 (-1.19659) | -1 | -1 |
| G: -6289.51193 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.04017 HOMO: -7.27360 LUMO: 0.88165 factor:1 | 1 (-1.16255) | 1 | 1 |
| G: -6289.51193 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.86632 HOMO: -6.84911 LUMO: 0.59865 factor:1 | 1 (-0.98870) | -1 | -1 |
| G: -6289.51193 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.26083 HOMO: -6.75114 LUMO: -2.49801 factor:1 | 1 (-1.38321) | -1 | -1 |
| G: -6289.51193 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.38555 HOMO: -6.97156 LUMO: 0.53606 factor:1 | 1 (-0.50793) | -1 | -1 |
| G: -6289.51193 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.45328 HOMO: -6.54434 LUMO: 0.73199 factor:1 | 1 (-0.57566) | -1 | -1 |
| G: -6289.51193 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.25058 HOMO: -6.21236 LUMO: 0.99866 factor:1 | 1 (-0.37296) | -1 | -1 |
| G: -6289.51193 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.45698 HOMO: -6.34025 LUMO: 0.50341 factor:1 | 1 (-0.57936) | -1 | -1 |
| G: -6289.51193 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.30566 HOMO: -6.59876 LUMO: -0.69389 factor:1 | 1 (-0.42804) | -1 | -1 |
| G: -6289.51193 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.44824 HOMO: -6.54978 LUMO: -1.00682 factor:1 | 1 (-0.57062) | -1 | -1 |
| G: -6289.51193 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.22242 HOMO: -6.82462 LUMO: -0.98777 factor:1 | 1 (-0.34480) | -1 | -1 |
| G: -6289.51193 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.42819 HOMO: -6.85455 LUMO: -0.68573 factor:1 | 1 (-0.55057) | -1 | -1 |
| G: -6289.51193 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.32177 HOMO: -7.55388 LUMO: -0.03265 factor:1 | 1 (-0.44414) | 1 | 1 |
| G: -6289.51193 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.26503 HOMO: -6.77019 LUMO: -0.71838 factor:1 | 1 (-0.38741) | -1 | -1 |
| G: -6289.51193 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.46318 HOMO: -6.84911 LUMO: -1.25444 factor:1 | 1 (-0.58556) | -1 | -1 |
| G: -6289.51193 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.29115 HOMO: -6.95251 LUMO: -1.03675 factor:1 | 1 (-0.41353) | -1 | -1 |
| G: -6289.51193 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.26315 HOMO: -6.80829 LUMO: -0.77280 factor:1 | 1 (-0.38553) | -1 | -1 |
| G: -6289.51193 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.31172 HOMO: -6.94162 LUMO: -0.94151 factor:1 | 1 (-0.43410) | -1 | -1 |
| G: -6289.51193 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.23423 HOMO: -6.89809 LUMO: -0.90886 factor:1 | 1 (-0.35661) | -1 | -1 |
| G: -6289.51193 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.36865 HOMO: -6.85183 LUMO: -0.88981 factor:1 | 1 (-0.49103) | -1 | -1 |
| G: -6289.51193 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.31276 HOMO: -6.51985 LUMO: -0.84627 factor:1 | 1 (-0.43514) | -1 | -1 |
| G: -6289.51193 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.51565 HOMO: -6.83278 LUMO: -1.08029 factor:1 | 1 (-0.63803) | -1 | -1 |
| G: -6289.51193 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.41026 HOMO: -6.91986 LUMO: 0.66396 factor:1 | 1 (-0.53264) | -1 | -1 |
| G: -6289.51193 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.28922 HOMO: -6.94162 LUMO: 0.50885 factor:1 | 1 (-0.41160) | -1 | -1 |
| G: -6289.51193 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12553.97528 HOMO: -6.94435 LUMO: 0.80546 factor:1 | 1 (-0.09766) | -1 | -1 |
| G: -6289.51193 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.20859 HOMO: -6.74298 LUMO: -0.81634 factor:1 | 1 (-0.33097) | -1 | -1 |
| G: -6289.51193 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.40326 HOMO: -7.04503 LUMO: 1.15921 factor:1 | 1 (-0.52564) | -1 | -1 |
| G: -6289.51193 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.19643 HOMO: -6.76475 LUMO: 0.75920 factor:1 | 1 (-0.31881) | -1 | -1 |
| G: -6289.51193 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.41047 HOMO: -7.05047 LUMO: 0.68845 factor:1 | 1 (-0.53285) | -1 | -1 |
| G: -6289.51193 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.32620 HOMO: -7.12666 LUMO: 0.60681 factor:1 | 1 (-0.44858) | 1 | 1 |
| G: -6289.51193 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.23409 HOMO: -6.90897 LUMO: -1.22723 factor:1 | 1 (-0.35647) | -1 | -1 |
| G: -6289.51193 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.43760 HOMO: -7.10761 LUMO: 0.58232 factor:1 | 1 (-0.55998) | 1 | 1 |
| G: -6289.51193 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.50642 HOMO: -6.57427 LUMO: 0.71294 factor:1 | 1 (-0.62880) | -1 | -1 |
| G: -6289.51193 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.96665 HOMO: -6.22597 LUMO: 0.99322 factor:1 | 1 (-1.08903) | -1 | -1 |
| G: -6289.51193 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.04978 HOMO: -6.83550 LUMO: -0.77825 factor:1 | 1 (-1.17216) | -1 | -1 |
| G: -6289.51193 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.90112 HOMO: -7.14843 LUMO: 0.44627 factor:1 | 1 (-1.02350) | 1 | 1 |
| G: -6289.51193 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.00159 HOMO: -7.08040 LUMO: 0.78913 factor:1 | 1 (-1.12397) | 1 | 1 |
| G: -6289.51193 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.08730 HOMO: -6.81373 LUMO: -0.93879 factor:1 | 1 (-1.20968) | -1 | -1 |
| G: -6289.51193 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.22344 HOMO: -6.95251 LUMO: 0.22585 factor:1 | 1 (-1.34582) | -1 | -1 |
| G: -6289.51193 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.36336 HOMO: -7.13483 LUMO: -1.25444 factor:1 | 1 (-1.48574) | -1 | -1 |
| G: -6289.51193 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.96719 HOMO: -6.37835 LUMO: -1.54289 factor:1 | 1 (-1.08957) | -1 | -1 |
| G: -6289.51193 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.45822 HOMO: -6.53617 LUMO: -1.43948 factor:1 | 1 (-1.58060) | -1 | -1 |
| G: -6289.51193 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12556.38678 HOMO: -6.38379 LUMO: 0.16055 factor:1 | 1 (-2.50916) | -1 | -1 |
| G: -6289.51193 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12556.16795 HOMO: -6.53617 LUMO: 0.15783 factor:1 | 1 (-2.29033) | -1 | -1 |
| G: -6289.51193 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12556.42335 HOMO: -6.79740 LUMO: -0.17960 factor:1 | 1 (-2.54573) | -1 | -1 |
| G: -6289.51193 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.50184 HOMO: -6.26678 LUMO: -0.41361 factor:1 | 1 (-1.62422) | -1 | -1 |
| G: -6289.51193 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12556.01902 HOMO: -6.35658 LUMO: -0.24218 factor:1 | 1 (-2.14140) | -1 | -1 |
| G: -6289.51193 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.41030 HOMO: -6.48175 LUMO: -0.71566 factor:1 | 1 (-1.53268) | -1 | -1 |
| G: -6289.51193 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12556.20528 HOMO: -6.21508 LUMO: -0.40001 factor:1 | 1 (-2.32766) | -1 | -1 |
| G: -6289.51193 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12556.26485 HOMO: -6.51985 LUMO: -0.32654 factor:1 | 1 (-2.38723) | -1 | -1 |
| G: -6289.51193 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.24129 HOMO: -6.45182 LUMO: -0.66396 factor:1 | 1 (-1.36367) | -1 | -1 |
| G: -6289.51193 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12556.05448 HOMO: -6.51441 LUMO: -0.65307 factor:1 | 1 (-2.17686) | -1 | -1 |
| G: -6289.51193 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.45700 HOMO: -6.57971 LUMO: -0.92519 factor:1 | 1 (-1.57938) | -1 | -1 |
| G: -6289.51193 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.27988 HOMO: -6.67223 LUMO: -0.58232 factor:1 | 1 (-1.40226) | -1 | -1 |
| G: -6289.51193 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.18823 HOMO: -6.10351 LUMO: -0.45987 factor:1 | 1 (-1.31061) | -1 | -1 |
| G: -6289.51193 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.34099 HOMO: -6.13889 LUMO: -0.50341 factor:1 | 1 (-1.46337) | -1 | -1 |
| G: -6289.51193 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.40932 HOMO: -6.63141 LUMO: -0.28300 factor:1 | 1 (-1.53170) | -1 | -1 |
| G: -6289.51193 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.26045 HOMO: -6.37563 LUMO: -0.22858 factor:1 | 1 (-1.38283) | -1 | -1 |
| G: -6289.51193 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.96940 HOMO: -6.37019 LUMO: 0.11429 factor:1 | 1 (-1.09178) | -1 | -1 |
| G: -6289.51193 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.46758 HOMO: -6.23957 LUMO: 0.28844 factor:1 | 1 (-1.58996) | -1 | -1 |
| G: -6289.51193 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.38114 HOMO: -6.41372 LUMO: -0.53879 factor:1 | 1 (-0.50352) | -1 | -1 |
| G: -6289.51193 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.39728 HOMO: -7.06680 LUMO: 0.32654 factor:1 | 1 (-0.51966) | 1 | 1 |
| G: -6289.51193 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.35328 HOMO: -6.50896 LUMO: -0.73743 factor:1 | 1 (-0.47566) | -1 | -1 |
| G: -6289.51193 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12553.98236 HOMO: -6.42189 LUMO: -0.28572 factor:1 | 1 (-0.10474) | -1 | -1 |
| G: -6289.51193 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.16582 HOMO: -6.79740 LUMO: -0.25851 factor:1 | 1 (-0.28820) | -1 | -1 |
| G: -6289.51193 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.25055 HOMO: -6.32393 LUMO: 0.17960 factor:1 | 1 (-0.37293) | -1 | -1 |
| G: -6289.51193 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12553.91675 HOMO: -6.65046 LUMO: 0.03537 factor:1 | 1 (-0.03913) | -1 | -1 |
| G: -6289.51193 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.11776 HOMO: -6.60148 LUMO: 0.07619 factor:1 | 1 (-0.24014) | -1 | -1 |
| G: -6289.51193 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.27458 HOMO: -6.57971 LUMO: 0.11429 factor:1 | 1 (-0.39696) | -1 | -1 |
| G: -6289.51193 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.17681 HOMO: -6.88448 LUMO: -1.21907 factor:1 | 1 (-0.29919) | -1 | -1 |
| G: -6289.51193 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.62326 HOMO: -6.97700 LUMO: 0.36463 factor:1 | 1 (-1.74564) | -1 | -1 |
| G: -6289.51193 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.35580 HOMO: -6.73210 LUMO: -0.84083 factor:1 | 1 (-1.47818) | -1 | -1 |
| G: -6289.51193 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12556.39514 HOMO: -6.21236 LUMO: -0.68845 factor:1 | 1 (-2.51752) | -1 | -1 |
| G: -6289.51193 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12556.30681 HOMO: -6.35658 LUMO: -0.82995 factor:1 | 1 (-2.42919) | -1 | -1 |
| G: -6289.51193 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12556.17853 HOMO: -6.75114 LUMO: -0.94424 factor:1 | 1 (-2.30091) | -1 | -1 |
| G: -6289.51193 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.19373 HOMO: -6.74026 LUMO: -1.46125 factor:1 | 1 (-1.31611) | -1 | -1 |
| G: -6289.51193 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12553.87792 HOMO: -7.06952 LUMO: 0.91974 factor:1 | 1 (-0.00030) | 1 | 1 |
| G: -6289.51193 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.09156 HOMO: -7.08857 LUMO: 0.74559 factor:1 | 1 (-0.21394) | 1 | 1 |
| G: -6289.51193 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.24691 HOMO: -6.74298 LUMO: 1.03131 factor:1 | 1 (-0.36929) | -1 | -1 |
| G: -6289.51193 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.83445 HOMO: -6.74842 LUMO: -1.77962 factor:1 | 1 (-1.95683) | -1 | -1 |
| G: -6289.51193 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.80266 HOMO: -6.82462 LUMO: -1.61908 factor:1 | 1 (-1.92504) | -1 | -1 |
| G: -6289.51193 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.00401 HOMO: -7.17020 LUMO: -1.02043 factor:1 | 1 (-1.12639) | -1 | -1 |
| G: -6289.51193 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.69183 HOMO: -6.26406 LUMO: -0.96328 factor:1 | 1 (-1.81421) | -1 | -1 |
| G: -6289.51193 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.87652 HOMO: -6.50896 LUMO: -0.38640 factor:1 | 1 (-0.99890) | -1 | -1 |
| G: -6289.51193 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.90262 HOMO: -7.27632 LUMO: -1.17553 factor:1 | 1 (-1.02500) | -1 | -1 |
| G: -6289.51193 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.88136 HOMO: -6.54162 LUMO: -1.36873 factor:1 | 1 (-2.00374) | -1 | -1 |
| G: -6289.51193 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.09870 HOMO: -6.42733 LUMO: -1.15648 factor:1 | 1 (-1.22108) | -1 | -1 |
| G: -6289.51193 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.11990 HOMO: -6.73754 LUMO: -2.58780 factor:1 | 1 (-1.24228) | -1 | -1 |
| G: -6289.51193 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.23016 HOMO: -7.20285 LUMO: 0.75103 factor:1 | 1 (-1.35254) | 1 | 1 |
| G: -6290.53967 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.24925 HOMO: -6.98788 LUMO: 0.34831 factor:1 | -1 (0.65612) | -1 | -1 |
| G: -6290.53967 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.74863 HOMO: -6.80013 LUMO: -1.11567 factor:1 | -1 (0.15674) | -1 | -1 |
| G: -6290.53967 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12556.64135 HOMO: -6.67767 LUMO: -0.82450 factor:1 | 1 (-1.73598) | -1 | -1 |
| G: -6290.53967 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12556.08155 HOMO: -6.84911 LUMO: -0.21497 factor:1 | 1 (-1.17618) | -1 | -1 |
| G: -6290.53967 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.70810 HOMO: -6.23141 LUMO: 0.21769 factor:1 | 1 (-0.80274) | -1 | -1 |
| G: -6290.53967 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.66202 HOMO: -6.68312 LUMO: 0.16327 factor:1 | -1 (0.24335) | -1 | -1 |
| G: -6290.53967 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.40056 HOMO: -7.04503 LUMO: -1.04220 factor:1 | 1 (-0.49519) | -1 | -1 |
| G: -6290.53967 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.48611 HOMO: -6.67495 LUMO: -0.71294 factor:1 | 1 (-0.58075) | -1 | -1 |
| G: -6290.53967 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12556.10906 HOMO: -6.70216 LUMO: -0.55239 factor:1 | 1 (-1.20370) | -1 | -1 |
| G: -6290.53967 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.41662 HOMO: -6.60420 LUMO: -0.71294 factor:1 | 1 (-0.51125) | -1 | -1 |
| G: -6290.53967 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.97246 HOMO: -7.40694 LUMO: 0.11973 factor:1 | 1 (-1.06709) | 1 | 1 |
| G: -6290.53967 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12556.00275 HOMO: -6.58788 LUMO: -0.29116 factor:1 | 1 (-1.09738) | -1 | -1 |
| G: -6290.53967 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.69451 HOMO: -6.63686 LUMO: -0.32654 factor:1 | -1 (0.21086) | -1 | -1 |
| G: -6290.53967 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12556.08310 HOMO: -6.85183 LUMO: -0.95512 factor:1 | 1 (-1.17774) | -1 | -1 |
| G: -6290.53967 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.54884 HOMO: -6.82189 LUMO: -0.88165 factor:1 | 1 (-0.64347) | -1 | -1 |
| G: -6290.53967 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.59148 HOMO: -6.97428 LUMO: -1.03947 factor:1 | 1 (-0.68611) | -1 | -1 |
| G: -6290.53967 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.59877 HOMO: -6.51441 LUMO: -0.05714 factor:1 | 1 (-0.69340) | -1 | -1 |
| G: -6290.53967 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.65365 HOMO: -6.61509 LUMO: -0.77008 factor:1 | 1 (-0.74829) | -1 | -1 |
| G: -6290.53967 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.71919 HOMO: -7.36340 LUMO: 0.29116 factor:1 | -1 (0.18618) | 1 | 1 |
| G: -6290.53967 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.70757 HOMO: -6.64230 LUMO: -0.79185 factor:1 | -1 (0.19780) | -1 | -1 |
| G: -6290.53967 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.61769 HOMO: -6.56883 LUMO: -1.03403 factor:1 | -1 (0.28768) | -1 | -1 |
| G: -6290.53967 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.72281 HOMO: -6.69400 LUMO: -0.77825 factor:1 | -1 (0.18256) | -1 | -1 |
| G: -6290.53967 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.70787 HOMO: -6.37019 LUMO: -0.79185 factor:1 | -1 (0.19750) | -1 | -1 |
| G: -6290.53967 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.46174 HOMO: -6.49808 LUMO: -0.94424 factor:1 | -1 (0.44363) | -1 | -1 |
| G: -6290.53967 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12556.68480 HOMO: -6.91713 LUMO: -0.75376 factor:1 | 1 (-1.77943) | -1 | -1 |
| G: -6290.53967 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.88345 HOMO: -7.13755 LUMO: 0.41361 factor:1 | 1 (-0.97809) | 1 | 1 |
| G: -6290.53967 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.54762 HOMO: -7.12122 LUMO: 0.39457 factor:1 | -1 (0.35775) | 1 | 1 |
| G: -6290.53967 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.96054 HOMO: -6.59332 LUMO: -0.57144 factor:1 | 1 (-1.05518) | -1 | -1 |
| G: -6290.53967 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12556.01973 HOMO: -6.62325 LUMO: -0.66940 factor:1 | 1 (-1.11436) | -1 | -1 |
| G: -6290.53967 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.38168 HOMO: -6.90897 LUMO: -0.08708 factor:1 | 1 (-0.47631) | -1 | -1 |
| G: -6290.53967 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.54633 HOMO: -6.65591 LUMO: -0.81090 factor:1 | 1 (-0.64096) | -1 | -1 |
| G: -6290.53967 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.49572 HOMO: -6.65318 LUMO: -0.94696 factor:1 | 1 (-0.59035) | -1 | -1 |
| G: -6290.53967 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.54122 HOMO: -6.96067 LUMO: -1.03675 factor:1 | -1 (0.36414) | -1 | -1 |
| G: -6290.53967 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.57461 HOMO: -6.23141 LUMO: -0.66396 factor:1 | -1 (0.33075) | -1 | -1 |
| G: -6290.53967 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.67320 HOMO: -6.52529 LUMO: -0.78369 factor:1 | -1 (0.23217) | -1 | -1 |
| G: -6290.53967 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.86651 HOMO: -6.39468 LUMO: -0.40817 factor:1 | -1 (0.03886) | -1 | -1 |
| G: -6290.53967 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.87571 HOMO: -6.76203 LUMO: -0.20409 factor:1 | -1 (0.02966) | -1 | -1 |
| G: -6290.53967 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.81622 HOMO: -6.96611 LUMO: -0.90342 factor:1 | -1 (0.08914) | -1 | -1 |
| G: -6290.53967 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.97568 HOMO: -6.54706 LUMO: -0.87893 factor:1 | 1 (-0.07031) | -1 | -1 |
| G: -6290.53967 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.78226 HOMO: -7.24367 LUMO: -0.97689 factor:1 | -1 (0.12310) | -1 | -1 |
| G: -6290.53967 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.38744 HOMO: -6.61781 LUMO: 1.43404 factor:1 | 1 (-0.48208) | -1 | -1 |
| G: -6290.53967 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.52130 HOMO: -6.17971 LUMO: 1.79867 factor:1 | 1 (-0.61593) | -1 | -1 |
| G: -6290.53967 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.29925 HOMO: -5.73344 LUMO: 2.13609 factor:1 | 1 (-0.39388) | -1 | -1 |
| G: -6290.53967 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.67130 HOMO: -6.72121 LUMO: 2.06807 factor:1 | -1 (0.23407) | -1 | -1 |
| G: -6290.53967 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.65012 HOMO: -6.91169 LUMO: 2.02997 factor:1 | -1 (0.25524) | -1 | -1 |
| G: -6290.53967 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.82164 HOMO: -7.06408 LUMO: 1.41499 factor:1 | -1 (0.08373) | 1 | 1 |
| G: -6290.53967 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.69924 HOMO: -6.94162 LUMO: -0.90070 factor:1 | -1 (0.20613) | -1 | -1 |
| G: -6290.53967 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.75658 HOMO: -7.09401 LUMO: 0.35103 factor:1 | -1 (0.14879) | 1 | 1 |
| G: -6290.53967 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.69048 HOMO: -6.78652 LUMO: 0.91974 factor:1 | -1 (0.21489) | -1 | -1 |
| G: -6290.53967 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.39765 HOMO: -6.32937 LUMO: -1.89119 factor:1 | 1 (-0.49228) | -1 | -1 |
| G: -6290.53967 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.60682 HOMO: -7.12666 LUMO: -1.06397 factor:1 | 1 (-0.70146) | -1 | -1 |
| G: -6290.53967 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.54734 HOMO: -6.38107 LUMO: -1.43132 factor:1 | 1 (-0.64197) | -1 | -1 |
| G: -6290.53967 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.77078 HOMO: -7.09129 LUMO: 0.08980 factor:1 | -1 (0.13459) | 1 | 1 |
| G: -6290.53967 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.25792 HOMO: -6.31304 LUMO: -0.57960 factor:1 | 1 (-0.35255) | -1 | -1 |
| G: -6290.53967 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.38347 HOMO: -6.94435 LUMO: -0.74287 factor:1 | 1 (-0.47810) | -1 | -1 |
| G: -6290.53967 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.34524 HOMO: -6.35658 LUMO: -1.53472 factor:1 | 1 (-0.43987) | -1 | -1 |
| G: -6290.53967 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.41803 HOMO: -6.39740 LUMO: -1.48846 factor:1 | 1 (-0.51266) | -1 | -1 |
| G: -6290.53967 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.18524 HOMO: -7.05319 LUMO: -0.33198 factor:1 | 1 (-0.27987) | -1 | -1 |
| G: -6290.53967 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.19827 HOMO: -6.68040 LUMO: -0.09252 factor:1 | 1 (-0.29290) | -1 | -1 |
| G: -6290.53967 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.47436 HOMO: -6.35930 LUMO: -0.43266 factor:1 | 1 (-0.56899) | -1 | -1 |
| G: -6290.53967 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12556.70061 HOMO: -6.59604 LUMO: -1.45853 factor:1 | 1 (-1.79524) | -1 | -1 |
| G: -6290.53967 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.93363 HOMO: -6.46270 LUMO: -1.49391 factor:1 | 1 (-1.02826) | -1 | -1 |
| G: -6290.53967 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.71648 HOMO: -7.05863 LUMO: -1.04764 factor:1 | 1 (-0.81112) | -1 | -1 |
| G: -6290.53967 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12556.07206 HOMO: -7.14027 LUMO: -0.81634 factor:1 | 1 (-1.16669) | -1 | -1 |
| G: -6290.53967 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.70281 HOMO: -6.80285 LUMO: -0.74287 factor:1 | -1 (0.20256) | -1 | -1 |
| G: -6290.53967 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12556.21807 HOMO: -6.53890 LUMO: -1.13471 factor:1 | 1 (-1.31270) | -1 | -1 |
| G: -6290.53967 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.67232 HOMO: -6.49808 LUMO: -1.35513 factor:1 | 1 (-0.76695) | -1 | -1 |
| G: -6290.53967 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.76468 HOMO: -6.75931 LUMO: -1.49663 factor:1 | -1 (0.14068) | -1 | -1 |
| G: -6290.53967 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.61064 HOMO: -6.84638 LUMO: -0.77552 factor:1 | -1 (0.29473) | -1 | -1 |
| G: -6290.53967 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.39020 HOMO: -6.65863 LUMO: -1.34696 factor:1 | -1 (0.51517) | -1 | -1 |
| G: -6290.53967 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.53635 HOMO: -6.25590 LUMO: -2.36467 factor:1 | -1 (0.36901) | -1 | -1 |
| G: -6290.53967 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.68678 HOMO: -7.24911 LUMO: 0.33470 factor:1 | -1 (0.21859) | 1 | 1 |
| G: -6290.53967 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.26336 HOMO: -6.65863 LUMO: -0.75648 factor:1 | 1 (-0.35799) | -1 | -1 |
| G: -6290.53967 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.31811 HOMO: -6.31576 LUMO: -0.83267 factor:1 | 1 (-0.41274) | -1 | -1 |
| G: -6290.53967 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.49142 HOMO: -6.64774 LUMO: -0.66124 factor:1 | 1 (-0.58605) | -1 | -1 |
| G: -6290.53967 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.65447 HOMO: -6.75387 LUMO: -1.00138 factor:1 | 1 (-0.74910) | -1 | -1 |
| G: -6290.53967 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.40562 HOMO: -6.52529 LUMO: -0.68301 factor:1 | 1 (-0.50025) | -1 | -1 |
| G: -6290.53967 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.35355 HOMO: -6.59332 LUMO: -0.68028 factor:1 | -1 (0.55182) | -1 | -1 |
| G: -6290.53967 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.34291 HOMO: -5.98650 LUMO: 0.31565 factor:1 | -1 (0.56246) | -1 | -1 |
| G: -6290.53967 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12556.55971 HOMO: -6.59876 LUMO: 0.22585 factor:1 | 1 (-1.65434) | -1 | -1 |
| G: -6290.53967 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.65673 HOMO: -6.72121 LUMO: 0.10340 factor:1 | 1 (-0.75136) | -1 | -1 |
| G: -6290.53967 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.31529 HOMO: -6.09807 LUMO: 0.20136 factor:1 | -1 (0.59008) | -1 | -1 |
| G: -6290.53967 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.92762 HOMO: -6.31576 LUMO: 0.06259 factor:1 | 1 (-1.02225) | -1 | -1 |
| G: -6290.53967 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12556.04014 HOMO: -6.35658 LUMO: -0.58232 factor:1 | 1 (-1.13477) | -1 | -1 |
| G: -6290.53967 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.26508 HOMO: -6.34842 LUMO: -0.55783 factor:1 | 1 (-0.35971) | -1 | -1 |
| G: -6290.53967 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.28399 HOMO: -6.47359 LUMO: -0.57144 factor:1 | 1 (-0.37862) | -1 | -1 |
| G: -6290.53967 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.66449 HOMO: -6.42189 LUMO: -0.09796 factor:1 | -1 (0.24088) | -1 | -1 |
| G: -6290.53967 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.76854 HOMO: -6.35658 LUMO: -0.31293 factor:1 | 1 (-0.86317) | -1 | -1 |
| G: -6290.53967 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.67120 HOMO: -7.35524 LUMO: 0.10340 factor:1 | 1 (-0.76584) | 1 | 1 |
| G: -6290.53967 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12556.20950 HOMO: -7.10217 LUMO: 0.36463 factor:1 | 1 (-1.30413) | 1 | 1 |
| G: -6290.53967 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.89138 HOMO: -6.43549 LUMO: -0.56872 factor:1 | -1 (0.01399) | -1 | -1 |
| G: -6290.53967 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.41596 HOMO: -6.50080 LUMO: -0.71294 factor:1 | 1 (-0.51059) | -1 | -1 |
| G: -6290.53967 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.24475 HOMO: -6.59060 LUMO: -0.57960 factor:1 | 1 (-0.33938) | -1 | -1 |
| G: -6290.53967 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.00872 HOMO: -6.78924 LUMO: -0.31565 factor:1 | 1 (-0.10335) | -1 | -1 |
| G: -6290.53967 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.95936 HOMO: -6.35658 LUMO: 0.07891 factor:1 | 1 (-0.05399) | -1 | -1 |
| G: -6290.53967 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.92877 HOMO: -6.74026 LUMO: -0.87621 factor:1 | 1 (-0.02340) | -1 | -1 |
| G: -6290.53967 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.12213 HOMO: -6.54434 LUMO: 0.81906 factor:1 | 1 (-0.21677) | -1 | -1 |
| G: -6290.53967 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.97280 HOMO: -6.66135 LUMO: 1.40955 factor:1 | 1 (-0.06743) | -1 | -1 |
| G: -6290.53967 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.79601 HOMO: -6.73754 LUMO: -2.54971 factor:1 | -1 (0.10936) | -1 | -1 |
| G: -6290.53967 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.84499 HOMO: -6.65318 LUMO: 0.69389 factor:1 | -1 (0.06038) | -1 | -1 |
| G: -6290.53967 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.54622 HOMO: -6.73482 LUMO: 0.62858 factor:1 | 1 (-0.64086) | -1 | -1 |
| G: -6290.53967 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.50007 HOMO: -6.83550 LUMO: 0.68573 factor:1 | 1 (-0.59470) | -1 | -1 |
| G: -6290.53967 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.36304 HOMO: -6.83278 LUMO: 0.45987 factor:1 | 1 (-0.45767) | -1 | -1 |
| G: -6290.53967 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.65281 HOMO: -6.78380 LUMO: 0.68301 factor:1 | 1 (-0.74744) | -1 | -1 |
| G: -6290.53967 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.49479 HOMO: -6.90625 LUMO: 1.36601 factor:1 | 1 (-0.58943) | -1 | -1 |
| G: -6290.53967 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.53417 HOMO: -6.82734 LUMO: 1.48302 factor:1 | 1 (-0.62880) | -1 | -1 |
| G: -6290.53967 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.63851 HOMO: -6.44094 LUMO: -0.94424 factor:1 | -1 (0.26686) | -1 | -1 |
| G: -6290.53967 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.46551 HOMO: -6.91441 LUMO: 0.28844 factor:1 | 1 (-0.56015) | -1 | -1 |
| G: -6290.53967 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.61232 HOMO: -6.49808 LUMO: -0.51157 factor:1 | 1 (-0.70695) | -1 | -1 |
| G: -6290.53967 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.45950 HOMO: -7.09673 LUMO: -0.06259 factor:1 | 1 (-0.55413) | 1 | 1 |
| G: -6290.53967 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.42383 HOMO: -6.77019 LUMO: 0.92247 factor:1 | 1 (-0.51846) | -1 | -1 |
| G: -6290.53967 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.69110 HOMO: -6.75931 LUMO: 1.13744 factor:1 | 1 (-0.78573) | -1 | -1 |
| G: -6290.53967 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.57724 HOMO: -6.15794 LUMO: 1.12383 factor:1 | 1 (-0.67188) | -1 | -1 |
| G: -6290.53967 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.68906 HOMO: -6.59604 LUMO: 1.19458 factor:1 | 1 (-0.78369) | -1 | -1 |
| G: -6290.53967 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.50249 HOMO: -7.09401 LUMO: 0.60137 factor:1 | 1 (-0.59713) | 1 | 1 |
| G: -6290.53967 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.61806 HOMO: -6.34025 LUMO: 0.48164 factor:1 | 1 (-0.71269) | -1 | -1 |
| G: -6290.53967 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.42007 HOMO: -6.72665 LUMO: -2.47624 factor:1 | 1 (-0.51470) | -1 | -1 |
| G: -6290.53967 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.34780 HOMO: -6.48175 LUMO: 0.58232 factor:1 | 1 (-0.44243) | -1 | -1 |
| G: -6290.53967 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.72836 HOMO: -6.94162 LUMO: 0.28300 factor:1 | -1 (0.17701) | -1 | -1 |
| G: -6290.53967 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.44113 HOMO: -6.65591 LUMO: 0.57144 factor:1 | 1 (-0.53576) | -1 | -1 |
| G: -6290.53967 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.36889 HOMO: -6.58788 LUMO: -1.03947 factor:1 | 1 (-0.46352) | -1 | -1 |
| G: -6290.53967 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.38940 HOMO: -7.18108 LUMO: 0.37824 factor:1 | 1 (-0.48404) | 1 | 1 |
| G: -6290.53967 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.48356 HOMO: -6.63958 LUMO: -1.52112 factor:1 | 1 (-0.57819) | -1 | -1 |
| G: -6290.53967 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.59907 HOMO: -6.12528 LUMO: -0.53606 factor:1 | 1 (-0.69370) | -1 | -1 |
| G: -6290.53967 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.71172 HOMO: -6.22324 LUMO: -0.87893 factor:1 | 1 (-0.80636) | -1 | -1 |
| G: -6290.53967 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.87701 HOMO: -6.62053 LUMO: -0.91974 factor:1 | -1 (0.02835) | -1 | -1 |
| G: -6290.53967 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.32080 HOMO: -6.84366 LUMO: -0.83811 factor:1 | 1 (-0.41544) | -1 | -1 |
| G: -6290.53967 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.98714 HOMO: -7.26000 LUMO: 0.25851 factor:1 | 1 (-0.08177) | 1 | 1 |
| G: -6290.53967 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.27427 HOMO: -6.49536 LUMO: -0.63403 factor:1 | 1 (-0.36890) | -1 | -1 |
| G: -6290.53967 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.02586 HOMO: -6.45726 LUMO: -0.77825 factor:1 | 1 (-0.12049) | -1 | -1 |
| G: -6290.53967 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.39237 HOMO: -6.74570 LUMO: -0.75103 factor:1 | 1 (-0.48700) | -1 | -1 |
| G: -6290.53967 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.46897 HOMO: -7.20285 LUMO: 0.10612 factor:1 | 1 (-0.56360) | 1 | 1 |
| G: -6290.53967 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.46252 HOMO: -6.45182 LUMO: -0.56600 factor:1 | 1 (-0.55715) | -1 | -1 |
| G: -6290.53967 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.44023 HOMO: -6.83278 LUMO: -0.71838 factor:1 | 1 (-0.53487) | -1 | -1 |
| G: -6290.53967 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.04311 HOMO: -7.01510 LUMO: -1.09662 factor:1 | 1 (-0.13774) | -1 | -1 |
| G: -6290.53967 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.00779 HOMO: -6.48719 LUMO: 0.16871 factor:1 | 1 (-0.10242) | -1 | -1 |
| G: -6290.53967 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.26616 HOMO: -7.30898 LUMO: 0.26667 factor:1 | 1 (-0.36080) | 1 | 1 |
| G: -6290.53967 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.14711 HOMO: -6.68856 LUMO: -0.78641 factor:1 | 1 (-0.24175) | -1 | -1 |
| G: -6290.53967 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.10635 HOMO: -6.56883 LUMO: -1.00682 factor:1 | 1 (-0.20098) | -1 | -1 |
| G: -6290.53967 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.73323 HOMO: -6.41100 LUMO: -0.48980 factor:1 | -1 (0.17214) | -1 | -1 |
| G: -6290.53967 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.92801 HOMO: -6.52257 LUMO: -0.59865 factor:1 | 1 (-0.02264) | -1 | -1 |
| G: -6290.53967 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.91440 HOMO: -6.63686 LUMO: -0.56055 factor:1 | 1 (-0.00903) | -1 | -1 |
| G: -6290.53967 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.85573 HOMO: -6.79740 LUMO: -0.75376 factor:1 | -1 (0.04963) | -1 | -1 |
| G: -6290.53967 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.48422 HOMO: -5.89127 LUMO: 0.22313 factor:1 | -1 (0.42115) | -1 | -1 |
| G: -6290.53967 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.99331 HOMO: -6.34842 LUMO: 0.11429 factor:1 | 1 (-0.08795) | -1 | -1 |
| G: -6290.53967 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.62117 HOMO: -6.13617 LUMO: 1.94834 factor:1 | -1 (0.28420) | -1 | -1 |
| G: -6290.53967 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.35904 HOMO: -6.50080 LUMO: 1.74153 factor:1 | 1 (-0.45367) | -1 | -1 |
| G: -6290.53967 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.89507 HOMO: -6.33481 LUMO: 1.68438 factor:1 | 1 (-0.98971) | -1 | -1 |
| G: -6290.53967 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.85657 HOMO: -6.53073 LUMO: 1.95106 factor:1 | 1 (-0.95120) | -1 | -1 |
| G: -6290.53967 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12556.42352 HOMO: -6.46270 LUMO: 1.89935 factor:1 | 1 (-1.51815) | -1 | -1 |
| G: -6290.53967 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12556.25546 HOMO: -5.87222 LUMO: 1.91568 factor:1 | 1 (-1.35009) | -1 | -1 |
| G: -6290.53967 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.93594 HOMO: -6.07630 LUMO: 1.81500 factor:1 | 1 (-1.03058) | -1 | -1 |
| G: -6290.53967 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.54247 HOMO: -6.20964 LUMO: 1.81500 factor:1 | 1 (-0.63710) | -1 | -1 |
| G: -6290.53967 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.85921 HOMO: -6.15522 LUMO: 1.90752 factor:1 | 1 (-0.95384) | -1 | -1 |
| G: -6290.53967 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.81126 HOMO: -6.11984 LUMO: 1.95378 factor:1 | 1 (-0.90589) | -1 | -1 |
| G: -6290.53967 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12556.06357 HOMO: -6.58516 LUMO: 2.04358 factor:1 | 1 (-1.15820) | -1 | -1 |
| G: -6290.53967 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12556.39748 HOMO: -7.37156 LUMO: 0.24490 factor:1 | 1 (-1.49211) | 1 | 1 |
| G: -6290.53967 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12556.39677 HOMO: -6.36474 LUMO: -0.90070 factor:1 | 1 (-1.49140) | -1 | -1 |
| G: -6290.53967 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12556.55440 HOMO: -6.43549 LUMO: -0.40817 factor:1 | 1 (-1.64904) | -1 | -1 |
| G: -6290.53967 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.91496 HOMO: -7.32258 LUMO: 0.29388 factor:1 | 1 (-1.00960) | 1 | 1 |
| G: -6290.53967 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12556.60692 HOMO: -6.41372 LUMO: -0.20409 factor:1 | 1 (-1.70156) | -1 | -1 |
| G: -6290.53967 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12556.45731 HOMO: -7.18381 LUMO: 0.42722 factor:1 | 1 (-1.55195) | 1 | 1 |
| G: -6290.53967 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.65442 HOMO: -6.53890 LUMO: -0.54151 factor:1 | 1 (-0.74905) | -1 | -1 |
| G: -6290.53967 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.88794 HOMO: -6.61509 LUMO: 0.08708 factor:1 | 1 (-0.98258) | -1 | -1 |
| G: -6290.53967 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12556.57098 HOMO: -6.78108 LUMO: 2.03541 factor:1 | 1 (-1.66561) | -1 | -1 |
| G: -6290.53967 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12556.44131 HOMO: -6.50896 LUMO: 1.53472 factor:1 | 1 (-1.53595) | -1 | -1 |
| G: -6290.53967 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12556.10923 HOMO: -6.65591 LUMO: 1.80411 factor:1 | 1 (-1.20386) | -1 | -1 |
| G: -6290.53967 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.84634 HOMO: -6.64502 LUMO: 1.52112 factor:1 | 1 (-0.94097) | -1 | -1 |
| G: -6290.53967 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.55694 HOMO: -6.72938 LUMO: 1.48030 factor:1 | 1 (-0.65158) | -1 | -1 |
| G: -6290.53967 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.41551 HOMO: -6.16882 LUMO: 1.96466 factor:1 | -1 (0.48986) | -1 | -1 |
| G: -6290.53967 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.28005 HOMO: -6.22597 LUMO: 1.43132 factor:1 | -1 (0.62532) | -1 | -1 |
| G: -6290.53967 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.44350 HOMO: -6.57699 LUMO: 2.05718 factor:1 | 1 (-0.53813) | -1 | -1 |
| G: -6290.53967 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.49281 HOMO: -6.52529 LUMO: 1.89663 factor:1 | 1 (-0.58744) | -1 | -1 |
| G: -6290.53967 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.68609 HOMO: -6.30760 LUMO: 1.88031 factor:1 | 1 (-0.78072) | -1 | -1 |
| G: -6290.53967 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.37958 HOMO: -6.14977 LUMO: 1.92657 factor:1 | 1 (-0.47421) | -1 | -1 |
| G: -6290.53967 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.79856 HOMO: -6.20964 LUMO: 1.83949 factor:1 | -1 (0.10680) | -1 | -1 |
| G: -6290.53967 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.65685 HOMO: -6.31848 LUMO: 1.91296 factor:1 | -1 (0.24852) | -1 | -1 |
| G: -6290.53967 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.57687 HOMO: -5.80691 LUMO: 2.19868 factor:1 | -1 (0.32850) | -1 | -1 |
| G: -6290.53967 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.75309 HOMO: -6.00827 LUMO: 2.15514 factor:1 | -1 (0.15227) | -1 | -1 |
| G: -6290.53967 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.74934 HOMO: -6.51713 LUMO: 2.08711 factor:1 | -1 (0.15603) | -1 | -1 |
| G: -6290.53967 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.45328 HOMO: -6.32937 LUMO: 2.11705 factor:1 | -1 (0.45209) | -1 | -1 |
| G: -6290.53967 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12556.04680 HOMO: -6.26678 LUMO: 1.95922 factor:1 | 1 (-1.14144) | -1 | -1 |
| G: -6290.53967 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12556.48874 HOMO: -6.43005 LUMO: 2.56603 factor:1 | 1 (-1.58338) | -1 | -1 |
| G: -6290.53967 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.55527 HOMO: -6.41644 LUMO: 2.68304 factor:1 | -1 (0.35010) | -1 | -1 |
| G: -6290.53967 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.89015 HOMO: -5.97834 LUMO: 2.02997 factor:1 | 1 (-0.98478) | -1 | -1 |
| G: -6290.53967 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.23318 HOMO: -6.14161 LUMO: 1.77690 factor:1 | 1 (-0.32782) | -1 | -1 |
| G: -6290.53967 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.55499 HOMO: -6.21508 LUMO: 1.80411 factor:1 | 1 (-0.64962) | -1 | -1 |
| G: -6290.53967 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12556.12569 HOMO: -6.46270 LUMO: 2.34562 factor:1 | 1 (-1.22032) | -1 | -1 |
| G: -6290.53967 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.77570 HOMO: -6.39195 LUMO: -0.75920 factor:1 | 1 (-0.87033) | -1 | -1 |
| G: -6290.53967 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.51722 HOMO: -7.08584 LUMO: -1.14016 factor:1 | 1 (-0.61185) | -1 | -1 |
| G: -6290.53967 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.43194 HOMO: -6.70216 LUMO: -0.65035 factor:1 | 1 (-0.52657) | -1 | -1 |
| G: -6290.53967 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.58217 HOMO: -6.79468 LUMO: -0.83811 factor:1 | 1 (-0.67680) | -1 | -1 |
| G: -6290.53967 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.21248 HOMO: -6.99877 LUMO: -0.79729 factor:1 | 1 (-0.30711) | -1 | -1 |
| G: -6290.53967 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.55833 HOMO: -7.08040 LUMO: -0.85444 factor:1 | 1 (-0.65296) | -1 | -1 |
| G: -6290.53967 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.85545 HOMO: -7.39333 LUMO: 0.12789 factor:1 | 1 (-0.95009) | 1 | 1 |
| G: -6290.53967 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.42883 HOMO: -7.05047 LUMO: 0.13878 factor:1 | 1 (-0.52347) | -1 | -1 |
| G: -6290.53967 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.27749 HOMO: -6.90897 LUMO: -0.77552 factor:1 | -1 (0.62788) | -1 | -1 |
| G: -6290.53967 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.46408 HOMO: -7.25456 LUMO: 0.05170 factor:1 | -1 (0.44129) | 1 | 1 |
| G: -6290.53967 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12553.99694 HOMO: -6.84638 LUMO: -0.84355 factor:1 | -1 (0.90842) | -1 | -1 |
| G: -6290.53967 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.56631 HOMO: -6.78108 LUMO: -0.81634 factor:1 | -1 (0.33905) | -1 | -1 |
| G: -6290.53967 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.33210 HOMO: -6.74570 LUMO: -0.77280 factor:1 | 1 (-0.42673) | -1 | -1 |
| G: -6290.53967 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.94101 HOMO: -7.28177 LUMO: -1.68438 factor:1 | 1 (-1.03564) | -1 | -1 |
| G: -6290.53967 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.48211 HOMO: -7.22190 LUMO: -1.63540 factor:1 | 1 (-0.57675) | -1 | -1 |
| G: -6290.53967 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.18861 HOMO: -7.15932 LUMO: -1.57554 factor:1 | 1 (-0.28324) | -1 | -1 |
| G: -6290.53967 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.86854 HOMO: -6.57971 LUMO: -0.93063 factor:1 | 1 (-0.96317) | -1 | -1 |
| G: -6290.53967 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.79665 HOMO: -6.88176 LUMO: 0.58232 factor:1 | 1 (-0.89128) | -1 | -1 |
| G: -6290.53967 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.95600 HOMO: -6.85727 LUMO: 0.51430 factor:1 | 1 (-1.05063) | -1 | -1 |
| G: -6290.53967 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.59431 HOMO: -6.83550 LUMO: 0.87893 factor:1 | 1 (-0.68894) | -1 | -1 |
| G: -6290.53967 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.42780 HOMO: -7.06680 LUMO: 0.87621 factor:1 | 1 (-0.52243) | 1 | 1 |
| G: -6290.53967 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.37030 HOMO: -6.52257 LUMO: 0.81362 factor:1 | 1 (-0.46493) | -1 | -1 |
| G: -6290.53967 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.71711 HOMO: -6.95523 LUMO: 1.17009 factor:1 | 1 (-0.81174) | -1 | -1 |
| G: -6290.53967 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.42543 HOMO: -7.21374 LUMO: 0.97145 factor:1 | 1 (-0.52006) | 1 | 1 |
| G: -6290.53967 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.78242 HOMO: -6.81373 LUMO: -1.54561 factor:1 | 1 (-0.87705) | -1 | -1 |
| G: -6290.53967 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.82971 HOMO: -6.86543 LUMO: -1.52656 factor:1 | 1 (-0.92434) | -1 | -1 |
| G: -6290.53967 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.97521 HOMO: -6.90081 LUMO: -0.78097 factor:1 | 1 (-1.06984) | -1 | -1 |
| G: -6290.53967 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.66103 HOMO: -6.64502 LUMO: -0.82723 factor:1 | 1 (-0.75566) | -1 | -1 |
| G: -6290.53967 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.51219 HOMO: -6.65591 LUMO: -0.82178 factor:1 | -1 (0.39318) | -1 | -1 |
| G: -6290.53967 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.43222 HOMO: -6.79468 LUMO: -1.46397 factor:1 | -1 (0.47315) | -1 | -1 |
| G: -6290.53967 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.61187 HOMO: -7.25728 LUMO: 0.73743 factor:1 | -1 (0.29350) | 1 | -1 |
| G: -6290.53967 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.32040 HOMO: -7.00149 LUMO: 1.30070 factor:1 | -1 (0.58496) | -1 | -1 |
| G: -6290.53967 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.59978 HOMO: -7.07768 LUMO: 0.78097 factor:1 | -1 (0.30558) | 1 | -1 |
| G: -6290.53967 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.40179 HOMO: -6.86271 LUMO: 0.86260 factor:1 | 1 (-0.49642) | -1 | -1 |
| G: -6290.53967 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.97271 HOMO: -6.94707 LUMO: 0.39729 factor:1 | 1 (-1.06734) | -1 | -1 |
| G: -6290.53967 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.34627 HOMO: -6.79740 LUMO: 0.67484 factor:1 | 1 (-0.44091) | -1 | -1 |
| G: -6290.53967 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12556.20109 HOMO: -6.91986 LUMO: -1.14288 factor:1 | 1 (-1.29572) | -1 | -1 |
| G: -6290.53967 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.54625 HOMO: -6.31576 LUMO: 1.01771 factor:1 | 1 (-0.64088) | -1 | -1 |
| G: -6290.53967 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.88593 HOMO: -6.81645 LUMO: 0.81362 factor:1 | 1 (-0.98056) | -1 | -1 |
| G: -6290.53967 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.32987 HOMO: -6.92258 LUMO: -0.99594 factor:1 | 1 (-0.42450) | -1 | -1 |
| G: -6290.53967 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.18616 HOMO: -6.81373 LUMO: 0.61770 factor:1 | 1 (-0.28079) | -1 | -1 |
| G: -6290.53967 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.41874 HOMO: -7.18653 LUMO: 1.19186 factor:1 | 1 (-0.51337) | 1 | 1 |
| G: -6290.53967 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.47463 HOMO: -7.00693 LUMO: 0.45715 factor:1 | 1 (-0.56926) | -1 | -1 |
| G: -6290.53967 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.20216 HOMO: -7.11306 LUMO: 0.53334 factor:1 | 1 (-0.29679) | 1 | 1 |
| G: -6290.53967 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.10755 HOMO: -6.63414 LUMO: -1.64357 factor:1 | 1 (-0.20218) | -1 | -1 |
| G: -6290.53967 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.89584 HOMO: -6.22052 LUMO: -0.74015 factor:1 | -1 (0.00952) | -1 | -1 |
| G: -6290.53967 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.05076 HOMO: -6.81101 LUMO: -0.50069 factor:1 | 1 (-0.14539) | -1 | -1 |
| G: -6290.53967 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.35009 HOMO: -6.71849 LUMO: -0.51974 factor:1 | -1 (0.55528) | -1 | -1 |
| G: -6290.53967 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.53429 HOMO: -6.72121 LUMO: -1.77690 factor:1 | -1 (0.37108) | -1 | -1 |
| G: -6290.53967 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.68240 HOMO: -6.94162 LUMO: -1.78779 factor:1 | -1 (0.22297) | -1 | -1 |
| G: -6290.53967 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.84537 HOMO: -6.91169 LUMO: 0.88981 factor:1 | -1 (0.06000) | -1 | -1 |
| G: -6290.53967 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.72025 HOMO: -6.97428 LUMO: 0.70750 factor:1 | -1 (0.18512) | -1 | -1 |
| G: -6290.53967 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.33523 HOMO: -6.74842 LUMO: 1.15921 factor:1 | -1 (0.57013) | -1 | -1 |
| G: -6290.53967 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.41393 HOMO: -7.25183 LUMO: -0.99594 factor:1 | -1 (0.49144) | -1 | -1 |
| G: -6290.53967 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.74822 HOMO: -6.43821 LUMO: -1.00410 factor:1 | -1 (0.15715) | -1 | -1 |
| G: -6290.53967 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.38854 HOMO: -6.52257 LUMO: -0.68573 factor:1 | -1 (0.51683) | -1 | -1 |
| G: -6290.53967 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.62724 HOMO: -6.60148 LUMO: -0.52518 factor:1 | -1 (0.27813) | -1 | -1 |
| G: -6290.53967 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.29366 HOMO: -6.07086 LUMO: -1.39594 factor:1 | -1 (0.61171) | -1 | -1 |
| G: -6290.53967 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.77864 HOMO: -6.78108 LUMO: -1.54833 factor:1 | -1 (0.12672) | -1 | -1 |
| G: -6290.53967 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.46397 HOMO: -6.73482 LUMO: -1.01498 factor:1 | -1 (0.44140) | -1 | -1 |
| G: -6290.53967 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.63271 HOMO: -6.85183 LUMO: 1.06669 factor:1 | -1 (0.27266) | -1 | -1 |
| G: -6290.53967 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.62936 HOMO: -6.98516 LUMO: 1.43948 factor:1 | -1 (0.27601) | -1 | -1 |
| G: -6290.53967 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.30228 HOMO: -6.94162 LUMO: 0.79185 factor:1 | -1 (0.60309) | -1 | -1 |
| G: -6290.53967 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.20144 HOMO: -6.67495 LUMO: -1.06669 factor:1 | -1 (0.70393) | -1 | -1 |
| G: -6290.53967 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.38955 HOMO: -6.88720 LUMO: -1.00682 factor:1 | -1 (0.51582) | -1 | -1 |
| G: -6290.53967 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.42691 HOMO: -6.85999 LUMO: -0.78097 factor:1 | -1 (0.47846) | -1 | -1 |
| G: -6290.53967 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.53001 HOMO: -6.51713 LUMO: -0.89798 factor:1 | -1 (0.37535) | -1 | -1 |
| G: -6290.53967 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.44019 HOMO: -6.63141 LUMO: -0.91430 factor:1 | -1 (0.46518) | -1 | -1 |
| G: -6290.53967 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.25118 HOMO: -6.63414 LUMO: 0.04354 factor:1 | -1 (0.65419) | -1 | -1 |
| G: -6290.53967 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.74692 HOMO: -6.65046 LUMO: -0.73743 factor:1 | -1 (0.15845) | -1 | -1 |
| G: -6290.53967 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.66773 HOMO: -6.73754 LUMO: -0.71838 factor:1 | -1 (0.23764) | -1 | -1 |
| G: -6290.53967 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.80055 HOMO: -6.65863 LUMO: -0.60137 factor:1 | -1 (0.10482) | -1 | -1 |
| G: -6290.53967 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.66735 HOMO: -6.61509 LUMO: -0.47892 factor:1 | -1 (0.23802) | -1 | -1 |
| G: -6290.53967 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.41320 HOMO: -6.82189 LUMO: -0.64763 factor:1 | -1 (0.49217) | -1 | -1 |
| G: -6290.53967 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.52378 HOMO: -6.56883 LUMO: -0.51974 factor:1 | -1 (0.38159) | -1 | -1 |
| G: -6290.53967 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.56373 HOMO: -6.97428 LUMO: -0.95512 factor:1 | -1 (0.34164) | -1 | -1 |
| G: -6290.53967 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.19877 HOMO: -6.70489 LUMO: -0.04082 factor:1 | -1 (0.70660) | -1 | -1 |
| G: -6290.53967 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.26500 HOMO: -6.74026 LUMO: 0.02177 factor:1 | -1 (0.64037) | -1 | -1 |
| G: -6290.53967 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.42604 HOMO: -6.50080 LUMO: -0.89525 factor:1 | -1 (0.47933) | -1 | -1 |
| G: -6290.53967 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.46571 HOMO: -6.46815 LUMO: -0.61226 factor:1 | -1 (0.43965) | -1 | -1 |
| G: -6290.53967 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.56142 HOMO: -6.57971 LUMO: -0.64219 factor:1 | -1 (0.34395) | -1 | -1 |
| G: -6290.53967 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.54381 HOMO: -7.17836 LUMO: 0.37280 factor:1 | -1 (0.36156) | 1 | 1 |
| G: -6290.53967 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.67834 HOMO: -6.67223 LUMO: 0.12245 factor:1 | -1 (0.22702) | -1 | -1 |
| G: -6290.53967 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.42332 HOMO: -6.55250 LUMO: 0.22858 factor:1 | -1 (0.48205) | -1 | -1 |
| G: -6290.53967 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.46095 HOMO: -6.97156 LUMO: -1.12927 factor:1 | -1 (0.44442) | -1 | -1 |
| G: -6290.53967 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.10170 HOMO: -6.78924 LUMO: -0.84900 factor:1 | 1 (-0.19633) | -1 | -1 |
| G: -6290.53967 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.20706 HOMO: -6.65046 LUMO: -0.65307 factor:1 | 1 (-0.30169) | -1 | -1 |
| G: -6290.53967 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.30053 HOMO: -7.41782 LUMO: 0.08980 factor:1 | 1 (-0.39516) | 1 | 1 |
| G: -6290.53967 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.34951 HOMO: -6.56339 LUMO: -0.68573 factor:1 | 1 (-0.44414) | -1 | -1 |
| G: -6290.53967 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.98787 HOMO: -6.31032 LUMO: -0.31837 factor:1 | 1 (-0.08250) | -1 | -1 |
| G: -6290.53967 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.99492 HOMO: -6.72938 LUMO: -0.45987 factor:1 | 1 (-0.08955) | -1 | -1 |
| G: -6290.53967 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.35988 HOMO: -6.59876 LUMO: -1.03131 factor:1 | 1 (-0.45451) | -1 | -1 |
| G: -6290.53967 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.15843 HOMO: -7.29265 LUMO: 0.29660 factor:1 | 1 (-0.25307) | 1 | 1 |
| G: -6290.53967 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.70421 HOMO: -6.42189 LUMO: -0.51157 factor:1 | 1 (-0.79884) | -1 | -1 |
| G: -6290.53967 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.80133 HOMO: -6.27767 LUMO: -0.52790 factor:1 | 1 (-0.89596) | -1 | -1 |
| G: -6290.53967 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12556.57601 HOMO: -6.41644 LUMO: -0.44627 factor:1 | 1 (-1.67064) | -1 | -1 |
| G: -6290.53967 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12556.55519 HOMO: -6.23413 LUMO: -0.52790 factor:1 | 1 (-1.64983) | -1 | -1 |
| G: -6290.53967 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.83722 HOMO: -6.63414 LUMO: -0.44082 factor:1 | 1 (-0.93185) | -1 | -1 |
| G: -6290.53967 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12556.40556 HOMO: -7.03142 LUMO: 0.47076 factor:1 | 1 (-1.50019) | -1 | -1 |
| G: -6290.53967 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12556.27206 HOMO: -6.62053 LUMO: -0.14422 factor:1 | 1 (-1.36669) | -1 | -1 |
| G: -6290.53967 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.60386 HOMO: -6.22324 LUMO: 1.96194 factor:1 | 1 (-0.69849) | -1 | -1 |
| G: -6290.53967 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12556.09045 HOMO: -6.17971 LUMO: 1.71704 factor:1 | 1 (-1.18508) | -1 | -1 |
| G: -6290.53967 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.45866 HOMO: -6.70761 LUMO: 1.68711 factor:1 | 1 (-0.55329) | -1 | -1 |
| G: -6290.53967 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.46579 HOMO: -6.52801 LUMO: 1.56193 factor:1 | 1 (-0.56042) | -1 | -1 |
| G: -6290.53967 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.36274 HOMO: -6.55794 LUMO: 1.52384 factor:1 | 1 (-0.45737) | -1 | -1 |
| G: -6290.53967 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.71178 HOMO: -6.47359 LUMO: 1.82316 factor:1 | 1 (-0.80641) | -1 | -1 |
| G: -6290.53967 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.39857 HOMO: -6.65863 LUMO: 1.83133 factor:1 | 1 (-0.49321) | -1 | -1 |
| G: -6290.53967 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.61440 HOMO: -6.46270 LUMO: 1.90208 factor:1 | -1 (0.29097) | -1 | -1 |
| G: -6290.53967 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.61851 HOMO: -6.41917 LUMO: 2.03269 factor:1 | -1 (0.28686) | -1 | -1 |
| G: -6290.53967 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.30334 HOMO: -6.48992 LUMO: 1.87486 factor:1 | -1 (0.60202) | -1 | -1 |
| G: -6290.53967 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.71309 HOMO: -6.51985 LUMO: 1.69527 factor:1 | -1 (0.19228) | -1 | -1 |
| G: -6290.53967 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.50000 HOMO: -6.36202 LUMO: 2.05718 factor:1 | -1 (0.40537) | -1 | -1 |
| G: -6290.53967 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.29050 HOMO: -5.96474 LUMO: 1.88575 factor:1 | -1 (0.61487) | -1 | -1 |
| G: -6290.53967 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.54531 HOMO: -6.56339 LUMO: 2.04630 factor:1 | -1 (0.36006) | -1 | -1 |
| G: -6290.53967 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.39230 HOMO: -6.43277 LUMO: 1.98371 factor:1 | -1 (0.51307) | -1 | -1 |
| G: -6290.53967 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.87047 HOMO: -6.53345 LUMO: 2.06262 factor:1 | 1 (-0.96511) | -1 | -1 |
| G: -6290.53967 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12556.40550 HOMO: -5.81779 LUMO: 2.11432 factor:1 | 1 (-1.50014) | -1 | -1 |
| G: -6290.53967 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.53828 HOMO: -5.91848 LUMO: 1.86942 factor:1 | 1 (-0.63291) | -1 | -1 |
| G: -6290.53967 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12556.52069 HOMO: -6.48447 LUMO: 1.70343 factor:1 | 1 (-1.61532) | -1 | -1 |
| G: -6290.53967 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12556.22874 HOMO: -6.29671 LUMO: -0.89525 factor:1 | 1 (-1.32337) | -1 | -1 |
| G: -6290.53967 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.26968 HOMO: -6.63414 LUMO: -0.76192 factor:1 | -1 (0.63569) | -1 | -1 |
| G: -6290.53967 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.48653 HOMO: -6.56883 LUMO: -0.86260 factor:1 | -1 (0.41884) | -1 | -1 |
| G: -6290.53967 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.27308 HOMO: -6.93074 LUMO: -0.27483 factor:1 | -1 (0.63228) | -1 | -1 |
| G: -6290.53967 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.87967 HOMO: -6.85999 LUMO: -0.01905 factor:1 | 1 (-0.97430) | -1 | -1 |
| G: -6290.53967 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.10967 HOMO: -6.26406 LUMO: 0.21769 factor:1 | 1 (-0.20430) | -1 | -1 |
| G: -6290.53967 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.28453 HOMO: -6.62325 LUMO: 0.31293 factor:1 | 1 (-0.37916) | -1 | -1 |
| G: -6290.53967 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12556.05744 HOMO: -6.59604 LUMO: 0.19592 factor:1 | 1 (-1.15208) | -1 | -1 |
| G: -6290.53967 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.19008 HOMO: -6.43277 LUMO: -0.27756 factor:1 | 1 (-0.28471) | -1 | -1 |
| G: -6290.53967 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.80177 HOMO: -6.54978 LUMO: -0.46531 factor:1 | 1 (-0.89640) | -1 | -1 |
| G: -6290.53967 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.96692 HOMO: -6.65046 LUMO: -0.15783 factor:1 | 1 (-0.06155) | -1 | -1 |
| G: -6290.53967 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.46219 HOMO: -7.28721 LUMO: 0.23946 factor:1 | 1 (-0.55683) | 1 | 1 |
| G: -6290.53967 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.51469 HOMO: -6.71849 LUMO: -0.56600 factor:1 | 1 (-0.60932) | -1 | -1 |
| G: -6290.53967 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.28654 HOMO: -6.85183 LUMO: -0.84355 factor:1 | 1 (-0.38118) | -1 | -1 |
| G: -6290.53967 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.33955 HOMO: -6.53345 LUMO: -0.84627 factor:1 | 1 (-0.43418) | -1 | -1 |
| G: -6290.53967 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.43308 HOMO: -6.60148 LUMO: -0.63130 factor:1 | 1 (-0.52771) | -1 | -1 |
| G: -6290.53967 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.27237 HOMO: -6.36202 LUMO: -0.60137 factor:1 | 1 (-0.36700) | -1 | -1 |
| G: -6290.53967 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.29114 HOMO: -6.28855 LUMO: -0.52790 factor:1 | 1 (-0.38578) | -1 | -1 |
| G: -6290.53967 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.09334 HOMO: -7.07224 LUMO: 0.41906 factor:1 | 1 (-0.18798) | 1 | 1 |
| G: -6290.53967 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.70125 HOMO: -6.36202 LUMO: -0.24218 factor:1 | 1 (-0.79588) | -1 | -1 |
| G: -6290.53967 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.47221 HOMO: -6.43549 LUMO: 0.14150 factor:1 | 1 (-0.56684) | -1 | -1 |
| G: -6290.53967 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.67575 HOMO: -6.76747 LUMO: -0.40545 factor:1 | 1 (-0.77038) | -1 | -1 |
| G: -6290.53967 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12556.24724 HOMO: -6.15249 LUMO: -0.51157 factor:1 | 1 (-1.34188) | -1 | -1 |
| G: -6290.53967 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.42998 HOMO: -6.33753 LUMO: -0.02993 factor:1 | 1 (-0.52461) | -1 | -1 |
| G: -6290.53967 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12556.02416 HOMO: -6.49808 LUMO: -0.83811 factor:1 | 1 (-1.11880) | -1 | -1 |
| G: -6290.53967 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.28502 HOMO: -6.64502 LUMO: -0.46259 factor:1 | 1 (-0.37965) | -1 | -1 |
| G: -6290.53967 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.44636 HOMO: -6.34570 LUMO: 0.22041 factor:1 | 1 (-0.54099) | -1 | -1 |
| G: -6290.53967 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.29955 HOMO: -6.63414 LUMO: -0.13606 factor:1 | 1 (-0.39418) | -1 | -1 |
| G: -6290.53967 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.13996 HOMO: -6.59604 LUMO: -0.79729 factor:1 | 1 (-0.23459) | -1 | -1 |
| G: -6290.53967 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.45069 HOMO: -7.09401 LUMO: 0.31837 factor:1 | -1 (0.45468) | 1 | 1 |
| G: -6290.53967 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.28729 HOMO: -6.48719 LUMO: -0.31021 factor:1 | -1 (0.61808) | -1 | -1 |
| G: -6290.53967 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.28609 HOMO: -7.11306 LUMO: 0.39729 factor:1 | -1 (0.61928) | 1 | 1 |
| G: -6290.53967 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.41619 HOMO: -6.95251 LUMO: 0.41089 factor:1 | -1 (0.48918) | -1 | -1 |
| G: -6290.53967 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.45989 HOMO: -6.61509 LUMO: -0.41906 factor:1 | -1 (0.44548) | -1 | -1 |
| G: -6290.53967 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.17227 HOMO: -6.25318 LUMO: -0.47348 factor:1 | -1 (0.73310) | -1 | -1 |
| G: -6290.53967 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.18378 HOMO: -6.77019 LUMO: -0.10340 factor:1 | -1 (0.72159) | -1 | -1 |
| G: -6290.53967 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.42408 HOMO: -6.54706 LUMO: -0.46259 factor:1 | -1 (0.48129) | -1 | -1 |
| G: -6290.53967 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.23956 HOMO: -6.34297 LUMO: -0.50341 factor:1 | -1 (0.66581) | -1 | -1 |
| G: -6290.53967 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.01452 HOMO: -6.20692 LUMO: -0.51974 factor:1 | -1 (0.89085) | -1 | -1 |
| G: -6290.53967 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.36002 HOMO: -7.03686 LUMO: 0.46804 factor:1 | -1 (0.54534) | -1 | -1 |
| G: -6290.53967 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.24974 HOMO: -6.47087 LUMO: 0.22585 factor:1 | -1 (0.65563) | -1 | -1 |
| G: -6290.53967 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.69458 HOMO: -6.41917 LUMO: 0.19320 factor:1 | 1 (-0.78921) | -1 | -1 |
| G: -6290.53967 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12556.54091 HOMO: -6.61237 LUMO: -0.04354 factor:1 | 1 (-1.63554) | -1 | -1 |
| G: -6290.53967 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.47561 HOMO: -6.56339 LUMO: 0.36735 factor:1 | 1 (-0.57024) | -1 | -1 |
| G: -6290.53967 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.17578 HOMO: -6.54978 LUMO: 1.12655 factor:1 | -1 (0.72959) | -1 | -1 |
| G: -6290.53967 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.32821 HOMO: -6.43277 LUMO: 1.17553 factor:1 | -1 (0.57715) | -1 | -1 |
| G: -6290.53967 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.30291 HOMO: -6.29944 LUMO: 1.40955 factor:1 | -1 (0.60246) | -1 | -1 |
| G: -6290.53967 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.90936 HOMO: -6.74842 LUMO: 0.74015 factor:1 | 1 (-1.00399) | -1 | -1 |
| G: -6290.53967 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.22799 HOMO: -6.15522 LUMO: 1.94289 factor:1 | 1 (-0.32262) | -1 | -1 |
| G: -6290.53967 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.76027 HOMO: -6.20147 LUMO: 1.40139 factor:1 | 1 (-0.85490) | -1 | -1 |
| G: -6290.53967 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.15008 HOMO: -6.41100 LUMO: 1.40139 factor:1 | 1 (-0.24471) | -1 | -1 |
| G: -6290.53967 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.30859 HOMO: -6.74570 LUMO: 1.80956 factor:1 | 1 (-0.40322) | -1 | -1 |
| G: -6290.53967 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12556.02985 HOMO: -6.60148 LUMO: -1.04764 factor:1 | 1 (-1.12448) | -1 | -1 |
| G: -6290.53967 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.39613 HOMO: -6.82734 LUMO: -0.83267 factor:1 | 1 (-0.49076) | -1 | -1 |
| G: -6290.53967 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12556.18607 HOMO: -7.01782 LUMO: -0.32382 factor:1 | 1 (-1.28070) | -1 | -1 |
| G: -6290.53967 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.23756 HOMO: -6.54434 LUMO: 0.11157 factor:1 | 1 (-0.33220) | -1 | -1 |
| G: -6290.53967 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.66379 HOMO: -6.53617 LUMO: 0.32926 factor:1 | -1 (0.24158) | -1 | -1 |
| G: -6290.53967 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.52811 HOMO: -6.62597 LUMO: -0.60137 factor:1 | -1 (0.37726) | -1 | -1 |
| G: -6290.53967 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.71554 HOMO: -6.60965 LUMO: -0.75376 factor:1 | -1 (0.18983) | -1 | -1 |
| G: -6290.53967 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.53162 HOMO: -6.29399 LUMO: 0.06803 factor:1 | -1 (0.37375) | -1 | -1 |
| G: -6290.53967 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.36748 HOMO: -6.60692 LUMO: -0.47076 factor:1 | -1 (0.53789) | -1 | -1 |
| G: -6290.53967 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.70226 HOMO: -7.33891 LUMO: 0.39184 factor:1 | -1 (0.20311) | 1 | 1 |
| G: -6290.53967 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.97987 HOMO: -6.60692 LUMO: 1.46125 factor:1 | 1 (-0.07450) | -1 | -1 |
| G: -6290.53967 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.93024 HOMO: -6.21780 LUMO: 2.09256 factor:1 | 1 (-0.02487) | -1 | -1 |
| G: -6290.53967 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.80942 HOMO: -6.28311 LUMO: 1.80411 factor:1 | -1 (0.09595) | -1 | -1 |
| G: -6290.53967 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.43570 HOMO: -6.51168 LUMO: 1.84765 factor:1 | -1 (0.46967) | -1 | -1 |
| G: -6290.53967 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.96667 HOMO: -6.66951 LUMO: 2.01636 factor:1 | 1 (-0.06131) | -1 | -1 |
| G: -6290.53967 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.70354 HOMO: -6.75387 LUMO: 1.73881 factor:1 | -1 (0.20183) | -1 | -1 |
| G: -6290.53967 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.84681 HOMO: -6.77291 LUMO: 1.89935 factor:1 | -1 (0.05856) | -1 | -1 |
| G: -6290.53967 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.75056 HOMO: -6.36474 LUMO: 1.61091 factor:1 | -1 (0.15481) | -1 | -1 |
| G: -6290.53967 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.85497 HOMO: -6.60420 LUMO: 1.40955 factor:1 | -1 (0.05040) | -1 | -1 |
| G: -6290.53967 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.87220 HOMO: -6.81645 LUMO: 1.59731 factor:1 | -1 (0.03317) | -1 | -1 |
| G: -6290.53967 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.69236 HOMO: -5.90215 LUMO: 2.12249 factor:1 | -1 (0.21301) | -1 | -1 |
| G: -6290.53967 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.53344 HOMO: -6.26950 LUMO: 1.62996 factor:1 | -1 (0.37193) | -1 | -1 |
| G: -6290.53967 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.70104 HOMO: -6.41100 LUMO: 1.80684 factor:1 | -1 (0.20433) | -1 | -1 |
| G: -6290.53967 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.68400 HOMO: -6.64230 LUMO: 2.23405 factor:1 | -1 (0.22136) | -1 | -1 |
| G: -6290.53967 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.37143 HOMO: -6.66951 LUMO: 2.21501 factor:1 | -1 (0.53394) | -1 | -1 |
| G: -6290.53967 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.71546 HOMO: -6.90897 LUMO: 2.00004 factor:1 | -1 (0.18991) | -1 | -1 |
| G: -6290.53967 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.74888 HOMO: -6.61781 LUMO: 1.42043 factor:1 | -1 (0.15649) | -1 | -1 |
| G: -6290.53967 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.37329 HOMO: -6.56611 LUMO: 1.60003 factor:1 | 1 (-0.46793) | -1 | -1 |
| G: -6290.53967 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.41319 HOMO: -6.70489 LUMO: 1.78779 factor:1 | 1 (-0.50782) | -1 | -1 |
| G: -6290.53967 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.61496 HOMO: -6.46815 LUMO: 1.59459 factor:1 | 1 (-0.70959) | -1 | -1 |
| G: -6290.53967 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.59529 HOMO: -6.31304 LUMO: 1.36873 factor:1 | 1 (-0.68992) | -1 | -1 |
| G: -6290.53967 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.52426 HOMO: -6.22597 LUMO: 1.54833 factor:1 | 1 (-0.61890) | -1 | -1 |
| G: -6290.53967 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.46176 HOMO: -5.63004 LUMO: 1.96466 factor:1 | 1 (-0.55639) | -1 | -1 |
| G: -6290.53967 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.80063 HOMO: -7.02598 LUMO: 1.79323 factor:1 | -1 (0.10474) | -1 | -1 |
| G: -6290.53967 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.93165 HOMO: -6.78924 LUMO: 2.10888 factor:1 | 1 (-0.02629) | -1 | -1 |
| G: -6290.53967 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.79171 HOMO: -6.13345 LUMO: 2.07351 factor:1 | -1 (0.11366) | -1 | -1 |
| G: -6290.53967 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.04488 HOMO: -6.46270 LUMO: -0.37552 factor:1 | 1 (-0.13951) | -1 | -1 |
| G: -6290.53967 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.32366 HOMO: -6.51985 LUMO: -0.49525 factor:1 | 1 (-0.41829) | -1 | -1 |
| G: -6290.53967 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.24480 HOMO: -6.60965 LUMO: 1.90480 factor:1 | 1 (-0.33943) | -1 | -1 |
| G: -6290.53967 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.30709 HOMO: -6.51168 LUMO: 1.92112 factor:1 | 1 (-0.40172) | -1 | -1 |
| G: -6290.53967 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.36823 HOMO: -6.71305 LUMO: 1.91024 factor:1 | 1 (-0.46287) | -1 | -1 |
| G: -6290.53967 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.25479 HOMO: -6.86815 LUMO: 2.02997 factor:1 | 1 (-0.34942) | -1 | -1 |
| G: -6290.53967 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.98858 HOMO: -6.69944 LUMO: 1.95106 factor:1 | 1 (-0.08321) | -1 | -1 |
| G: -6290.53967 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.49531 HOMO: -6.45182 LUMO: 1.66806 factor:1 | 1 (-0.58994) | -1 | -1 |
| G: -6290.53967 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.42979 HOMO: -6.44638 LUMO: 2.16058 factor:1 | 1 (-0.52442) | -1 | -1 |
| G: -6290.53967 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.28491 HOMO: -6.65591 LUMO: 1.95106 factor:1 | 1 (-0.37954) | -1 | -1 |
| G: -6290.53967 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.09043 HOMO: -6.35114 LUMO: 1.42316 factor:1 | 1 (-0.18506) | -1 | -1 |
| G: -6290.53967 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.10589 HOMO: -6.48719 LUMO: 1.59187 factor:1 | 1 (-0.20052) | -1 | -1 |
| G: -6290.53967 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.33610 HOMO: -7.05591 LUMO: 1.61908 factor:1 | 1 (-0.43073) | -1 | -1 |
| G: -6290.53967 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.36807 HOMO: -6.92258 LUMO: 1.87214 factor:1 | 1 (-0.46270) | -1 | -1 |
| G: -6290.53967 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.10679 HOMO: -5.85861 LUMO: 2.11705 factor:1 | 1 (-0.20142) | -1 | -1 |
| G: -6290.53967 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.94224 HOMO: -6.27767 LUMO: 1.75513 factor:1 | 1 (-0.03687) | -1 | -1 |
| G: -6290.53967 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.29370 HOMO: -6.16882 LUMO: 1.73881 factor:1 | 1 (-0.38833) | -1 | -1 |
| G: -6290.53967 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.35142 HOMO: -6.62053 LUMO: 1.39594 factor:1 | 1 (-0.44605) | -1 | -1 |
| G: -6290.53967 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.63042 HOMO: -5.46405 LUMO: 1.68166 factor:1 | -1 (0.27494) | -1 | -1 |
| G: -6290.53967 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.56806 HOMO: -6.39740 LUMO: 1.68711 factor:1 | -1 (0.33731) | -1 | -1 |
| G: -6290.53967 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.39341 HOMO: -6.99333 LUMO: 2.08439 factor:1 | -1 (0.51196) | -1 | -1 |
| G: -6290.53967 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.21458 HOMO: -6.16882 LUMO: 1.71976 factor:1 | -1 (0.69079) | -1 | -1 |
| G: -6290.53967 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.14043 HOMO: -7.19741 LUMO: 2.24766 factor:1 | -1 (0.76494) | 1 | 1 |
| G: -6290.53967 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.77296 HOMO: -6.77291 LUMO: 2.17691 factor:1 | -1 (0.13241) | -1 | -1 |
| G: -6290.53967 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.45850 HOMO: -6.29944 LUMO: 2.16603 factor:1 | -1 (0.44687) | -1 | -1 |
| G: -6290.53967 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.61687 HOMO: -6.10079 LUMO: 1.83949 factor:1 | -1 (0.28850) | -1 | -1 |
| G: -6290.53967 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.70006 HOMO: -6.63686 LUMO: 2.05990 factor:1 | -1 (0.20531) | -1 | -1 |
| G: -6290.53967 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.50748 HOMO: -6.91713 LUMO: 1.87486 factor:1 | -1 (0.39788) | -1 | -1 |
| G: -6290.53967 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.34389 HOMO: -6.63958 LUMO: 1.79323 factor:1 | -1 (0.56148) | -1 | -1 |
| G: -6290.53967 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.59108 HOMO: -6.61781 LUMO: 1.70071 factor:1 | -1 (0.31429) | -1 | -1 |
| G: -6290.53967 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.49173 HOMO: -6.20420 LUMO: 1.82861 factor:1 | -1 (0.41364) | -1 | -1 |
| G: -6290.53967 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.62348 HOMO: -6.47903 LUMO: -2.16875 factor:1 | -1 (0.28188) | -1 | -1 |
| G: -6290.53967 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.41907 HOMO: -6.53073 LUMO: 2.18235 factor:1 | -1 (0.48629) | -1 | -1 |
| G: -6290.53967 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.27417 HOMO: -7.01782 LUMO: 1.72520 factor:1 | -1 (0.63120) | -1 | -1 |
| G: -6290.53967 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.55823 HOMO: -6.66135 LUMO: -0.75648 factor:1 | -1 (0.34714) | -1 | -1 |
| G: -6290.53967 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.24412 HOMO: -7.56749 LUMO: 0.22585 factor:1 | 1 (-0.33875) | 1 | 1 |
| G: -6290.53967 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.28050 HOMO: -6.45182 LUMO: -0.71294 factor:1 | 1 (-0.37514) | -1 | -1 |
| G: -6290.53967 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.20548 HOMO: -6.31032 LUMO: -0.34286 factor:1 | 1 (-0.30011) | -1 | -1 |
| G: -6290.53967 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.85255 HOMO: -6.41917 LUMO: 2.04085 factor:1 | -1 (0.05282) | -1 | -1 |
| G: -6290.53967 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.27327 HOMO: -6.61781 LUMO: 1.98915 factor:1 | 1 (-0.36790) | -1 | -1 |
| G: -6290.53967 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.07533 HOMO: -5.86405 LUMO: 1.57282 factor:1 | 1 (-0.16996) | -1 | -1 |
| G: -6290.53967 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.75056 HOMO: -6.44094 LUMO: 1.80956 factor:1 | -1 (0.15481) | -1 | -1 |
| G: -6290.53967 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.52359 HOMO: -6.59060 LUMO: 2.08167 factor:1 | -1 (0.38178) | -1 | -1 |
| G: -6290.53967 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.60291 HOMO: -6.20147 LUMO: 1.69799 factor:1 | -1 (0.30245) | -1 | -1 |
| G: -6290.53967 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.25371 HOMO: -6.50352 LUMO: -0.41361 factor:1 | -1 (0.65166) | -1 | -1 |
| G: -6290.53967 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.67540 HOMO: -6.10896 LUMO: -0.55783 factor:1 | -1 (0.22996) | -1 | -1 |
| G: -6290.53967 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.34794 HOMO: -6.74842 LUMO: -0.56872 factor:1 | -1 (0.55743) | -1 | -1 |
| G: -6290.53967 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.19618 HOMO: -6.59060 LUMO: -0.22041 factor:1 | -1 (0.70918) | -1 | -1 |
| G: -6290.53967 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.47156 HOMO: -6.22052 LUMO: -0.60137 factor:1 | -1 (0.43380) | -1 | -1 |
| G: -6290.53967 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.44552 HOMO: -6.65863 LUMO: 0.07891 factor:1 | -1 (0.45985) | -1 | -1 |
| G: -6290.53967 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.63059 HOMO: -6.57427 LUMO: 1.71160 factor:1 | -1 (0.27478) | -1 | -1 |
| G: -6290.53967 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.74634 HOMO: -5.84773 LUMO: 1.99459 factor:1 | -1 (0.15902) | -1 | -1 |
| G: -6290.53967 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.83247 HOMO: -6.02188 LUMO: 1.91296 factor:1 | -1 (0.07290) | -1 | -1 |
| G: -6290.53967 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.58528 HOMO: -6.17698 LUMO: 2.00004 factor:1 | -1 (0.32009) | -1 | -1 |
| G: -6290.53967 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.54672 HOMO: -6.02732 LUMO: 1.90752 factor:1 | -1 (0.35865) | -1 | -1 |
| G: -6290.53967 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.42247 HOMO: -6.68584 LUMO: -0.50885 factor:1 | -1 (0.48289) | -1 | -1 |
| G: -6290.53967 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.54158 HOMO: -6.61781 LUMO: -0.73471 factor:1 | -1 (0.36379) | -1 | -1 |
| G: -6290.53967 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.55548 HOMO: -6.66407 LUMO: -0.79729 factor:1 | -1 (0.34988) | -1 | -1 |
| G: -6290.53967 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.29717 HOMO: -6.56339 LUMO: 0.23130 factor:1 | -1 (0.60820) | -1 | -1 |
| G: -6290.53967 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.61508 HOMO: -6.76747 LUMO: 0.08980 factor:1 | -1 (0.29029) | -1 | -1 |
| G: -6290.53967 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.26838 HOMO: -6.70489 LUMO: -0.53334 factor:1 | -1 (0.63699) | -1 | -1 |
| G: -6290.53967 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.37134 HOMO: -7.28993 LUMO: 0.10885 factor:1 | -1 (0.53402) | 1 | 1 |
| G: -6290.53967 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.18625 HOMO: -6.22052 LUMO: 0.51974 factor:1 | -1 (0.71912) | -1 | -1 |
| G: -6290.53967 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.00451 HOMO: -6.81645 LUMO: 0.25307 factor:1 | -1 (0.90086) | -1 | -1 |
| G: -6290.53967 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.50678 HOMO: -6.80285 LUMO: 0.02721 factor:1 | -1 (0.39859) | -1 | -1 |
| G: -6290.53967 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.17507 HOMO: -6.51441 LUMO: 0.08163 factor:1 | -1 (0.73030) | -1 | -1 |
| G: -6290.53967 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.76575 HOMO: -6.73482 LUMO: -0.77008 factor:1 | -1 (0.13962) | -1 | -1 |
| G: -6290.53967 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.65780 HOMO: -6.29127 LUMO: -0.44355 factor:1 | -1 (0.24757) | -1 | -1 |
| G: -6290.53967 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.14975 HOMO: -6.72938 LUMO: -0.64763 factor:1 | 1 (-0.24439) | -1 | -1 |
| G: -6290.53967 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.18023 HOMO: -6.49264 LUMO: -0.74559 factor:1 | 1 (-0.27486) | -1 | -1 |
| G: -6290.53967 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.04140 HOMO: -6.67223 LUMO: -0.55239 factor:1 | 1 (-0.13603) | -1 | -1 |
| G: -6290.53967 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.36113 HOMO: -6.33481 LUMO: 0.33198 factor:1 | 1 (-0.45576) | -1 | -1 |
| G: -6290.53967 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.41039 HOMO: -6.76475 LUMO: -0.25307 factor:1 | -1 (0.49498) | -1 | -1 |
| G: -6290.53967 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.26166 HOMO: -6.65318 LUMO: 0.03810 factor:1 | -1 (0.64371) | -1 | -1 |
| G: -6290.53967 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12553.97194 HOMO: -6.09263 LUMO: 0.21497 factor:1 | -1 (0.93343) | -1 | -1 |
| G: -6290.53967 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.07330 HOMO: -6.32120 LUMO: -0.85444 factor:1 | -1 (0.83207) | -1 | -1 |
| G: -6290.53967 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12553.76902 HOMO: -6.57155 LUMO: -0.67484 factor:1 | -1 (1.13635) | -1 | -1 |
| G: -6290.53967 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12553.41067 HOMO: -6.53345 LUMO: -0.78913 factor:1 | -1 (1.49469) | -1 | -1 |
| G: -6290.53967 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.17548 HOMO: -7.07768 LUMO: 0.28844 factor:1 | -1 (0.72989) | 1 | 1 |
| G: -6290.53967 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.85171 HOMO: -6.75114 LUMO: 0.18776 factor:1 | -1 (0.05366) | -1 | -1 |
| G: -6290.53967 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.72523 HOMO: -6.77019 LUMO: -0.12245 factor:1 | -1 (0.18014) | -1 | -1 |
| G: -6290.53967 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.63233 HOMO: -6.43549 LUMO: 0.16327 factor:1 | -1 (0.27304) | -1 | -1 |
| G: -6290.53967 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.82349 HOMO: -6.69400 LUMO: -0.16327 factor:1 | -1 (0.08188) | -1 | -1 |
| G: -6290.53967 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.54321 HOMO: -6.38651 LUMO: -0.61770 factor:1 | -1 (0.36216) | -1 | -1 |
| G: -6290.53967 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.64433 HOMO: -6.34297 LUMO: -0.33198 factor:1 | -1 (0.26104) | -1 | -1 |
| G: -6290.53967 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.39890 HOMO: -7.51578 LUMO: 0.02177 factor:1 | 1 (-0.49353) | 1 | 1 |
| G: -6290.53967 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.51724 HOMO: -6.47359 LUMO: -0.22585 factor:1 | 1 (-0.61188) | -1 | -1 |
| G: -6290.53967 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.55733 HOMO: -6.68040 LUMO: -0.47076 factor:1 | 1 (-0.65196) | -1 | -1 |
| G: -6290.53967 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.30592 HOMO: -6.75659 LUMO: -0.57688 factor:1 | 1 (-0.40055) | -1 | -1 |
| G: -6290.53967 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.35501 HOMO: -6.73754 LUMO: -0.61226 factor:1 | 1 (-0.44964) | -1 | -1 |
| G: -6290.53967 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.73402 HOMO: -7.37429 LUMO: 0.31293 factor:1 | -1 (0.17135) | 1 | 1 |
| G: -6290.53967 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.80036 HOMO: -6.23413 LUMO: -0.90886 factor:1 | -1 (0.10501) | -1 | -1 |
| G: -6290.53967 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.63363 HOMO: -6.51985 LUMO: -0.68028 factor:1 | -1 (0.27173) | -1 | -1 |
| G: -6290.53967 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.52204 HOMO: -6.52257 LUMO: -0.77280 factor:1 | -1 (0.38333) | -1 | -1 |
| G: -6290.53967 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.42841 HOMO: -7.29537 LUMO: 0.31837 factor:1 | -1 (0.47696) | 1 | 1 |
| G: -6290.53967 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.35205 HOMO: -6.08447 LUMO: 0.25851 factor:1 | -1 (0.55332) | -1 | -1 |
| G: -6290.53967 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.38996 HOMO: -6.20964 LUMO: 0.13606 factor:1 | -1 (0.51541) | -1 | -1 |
| G: -6290.53967 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.11594 HOMO: -6.49808 LUMO: -0.14150 factor:1 | -1 (0.78943) | -1 | -1 |
| G: -6290.53967 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.48307 HOMO: -7.10761 LUMO: 0.28028 factor:1 | -1 (0.42229) | 1 | 1 |
| G: -6290.53967 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.35400 HOMO: -6.60965 LUMO: -0.62858 factor:1 | 1 (-0.44863) | -1 | -1 |
| G: -6290.53967 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.54952 HOMO: -6.40012 LUMO: -0.26939 factor:1 | 1 (-0.64415) | -1 | -1 |
| G: -6290.53967 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.08924 HOMO: -6.65318 LUMO: -0.73199 factor:1 | 1 (-0.18387) | -1 | -1 |
| G: -6290.53967 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.51860 HOMO: -6.51441 LUMO: -0.44899 factor:1 | 1 (-0.61324) | -1 | -1 |
| G: -6290.53967 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.36355 HOMO: -6.28583 LUMO: -0.48708 factor:1 | 1 (-0.45819) | -1 | -1 |
| G: -6290.53967 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.80575 HOMO: -6.96884 LUMO: 0.19864 factor:1 | -1 (0.09962) | -1 | -1 |
| G: -6290.53967 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.54626 HOMO: -6.89809 LUMO: 0.34558 factor:1 | -1 (0.35911) | -1 | -1 |
| G: -6290.53967 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.68245 HOMO: -6.67495 LUMO: -0.15510 factor:1 | -1 (0.22292) | -1 | -1 |
| G: -6290.53967 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.37311 HOMO: -7.34980 LUMO: 0.19864 factor:1 | -1 (0.53225) | 1 | 1 |
| G: -6290.53967 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.17839 HOMO: -6.71305 LUMO: -0.81634 factor:1 | -1 (0.72698) | -1 | -1 |
| G: -6290.53967 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.39826 HOMO: -6.39468 LUMO: -0.47076 factor:1 | -1 (0.50711) | -1 | -1 |
| G: -6290.53967 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.60539 HOMO: -6.31304 LUMO: 1.39594 factor:1 | -1 (0.29998) | -1 | -1 |
| G: -6290.53967 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.75625 HOMO: -6.57155 LUMO: 1.55105 factor:1 | -1 (0.14912) | -1 | -1 |
| G: -6290.53967 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.44792 HOMO: -6.68312 LUMO: 1.69255 factor:1 | -1 (0.45745) | -1 | -1 |
| G: -6290.53967 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.55932 HOMO: -6.61509 LUMO: 1.73881 factor:1 | -1 (0.34605) | -1 | -1 |
| G: -6290.53967 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.62261 HOMO: -6.17971 LUMO: 1.90208 factor:1 | -1 (0.28275) | -1 | -1 |
| G: -6290.53967 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.19605 HOMO: -6.53073 LUMO: 1.73337 factor:1 | -1 (0.70932) | -1 | -1 |
| G: -6290.53967 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.19891 HOMO: -5.91303 LUMO: 1.90480 factor:1 | -1 (0.70646) | -1 | -1 |
| G: -6290.53967 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12553.93044 HOMO: -6.42733 LUMO: 1.80139 factor:1 | -1 (0.97493) | -1 | -1 |
| G: -6290.53967 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.33929 HOMO: -6.78924 LUMO: 2.31569 factor:1 | -1 (0.56608) | -1 | -1 |
| G: -6290.53967 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.55102 HOMO: -6.04093 LUMO: 1.91568 factor:1 | -1 (0.35435) | -1 | -1 |
| G: -6290.53967 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.54346 HOMO: -6.90081 LUMO: 2.36739 factor:1 | -1 (0.36191) | -1 | -1 |
| G: -6290.53967 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.52451 HOMO: -6.60965 LUMO: 2.18507 factor:1 | 1 (-0.61914) | -1 | -1 |
| G: -6290.53967 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.58799 HOMO: -6.75387 LUMO: 2.48712 factor:1 | 1 (-0.68262) | -1 | -1 |
| G: -6290.53967 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.34230 HOMO: -6.56883 LUMO: 1.71432 factor:1 | 1 (-0.43693) | -1 | -1 |
| G: -6290.53967 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.37732 HOMO: -6.41644 LUMO: 1.72792 factor:1 | 1 (-0.47195) | -1 | -1 |
| G: -6290.53967 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.20799 HOMO: -6.92530 LUMO: 2.54426 factor:1 | 1 (-0.30262) | -1 | -1 |
| G: -6290.53967 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.24102 HOMO: -6.41644 LUMO: 2.70209 factor:1 | 1 (-0.33565) | -1 | -1 |
| G: -6290.53967 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.19558 HOMO: -6.29671 LUMO: 2.14698 factor:1 | 1 (-0.29021) | -1 | -1 |
| G: -6290.53967 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.38140 HOMO: -6.29127 LUMO: 1.87486 factor:1 | 1 (-0.47604) | -1 | -1 |
| G: -6290.53967 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.28284 HOMO: -6.75931 LUMO: 2.78917 factor:1 | 1 (-0.37748) | -1 | -1 |
| G: -6290.53967 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.01748 HOMO: -6.40828 LUMO: 1.86942 factor:1 | 1 (-0.11211) | -1 | -1 |
| G: -6290.53967 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.35865 HOMO: -6.45726 LUMO: 1.97010 factor:1 | 1 (-0.45329) | -1 | -1 |
| G: -6290.53967 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.25729 HOMO: -6.43277 LUMO: 1.22723 factor:1 | 1 (-0.35192) | -1 | -1 |
| G: -6290.53967 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.27884 HOMO: -6.63414 LUMO: 1.62452 factor:1 | 1 (-0.37348) | -1 | -1 |
| G: -6290.53967 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.10858 HOMO: -6.54162 LUMO: 2.16058 factor:1 | 1 (-0.20321) | -1 | -1 |
| G: -6290.53967 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.32355 HOMO: -6.40284 LUMO: 1.88575 factor:1 | 1 (-0.41818) | -1 | -1 |
| G: -6290.53967 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.35972 HOMO: -6.20964 LUMO: 1.84221 factor:1 | 1 (-0.45435) | -1 | -1 |
| G: -6290.53967 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.51466 HOMO: -6.58516 LUMO: 1.69799 factor:1 | 1 (-0.60929) | -1 | -1 |
| G: -6290.53967 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.34935 HOMO: -6.44094 LUMO: 2.05446 factor:1 | 1 (-0.44398) | -1 | -1 |
| G: -6290.53967 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.16924 HOMO: -6.61509 LUMO: 2.16058 factor:1 | 1 (-0.26387) | -1 | -1 |
| G: -6290.53967 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.10091 HOMO: -6.65591 LUMO: 1.69527 factor:1 | 1 (-0.19554) | -1 | -1 |
| G: -6290.53967 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.39294 HOMO: -5.55112 LUMO: 1.80411 factor:1 | 1 (-0.48757) | -1 | -1 |
| G: -6290.53967 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.40271 HOMO: -6.68312 LUMO: 2.38100 factor:1 | 1 (-0.49734) | -1 | -1 |
| G: -6290.53967 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.43825 HOMO: -6.51168 LUMO: 2.14698 factor:1 | 1 (-0.53288) | -1 | -1 |
| G: -6290.53967 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.23220 HOMO: -6.04637 LUMO: 1.48302 factor:1 | 1 (-0.32684) | -1 | -1 |
| G: -6290.53967 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.40211 HOMO: -6.81645 LUMO: -0.74287 factor:1 | 1 (-0.49674) | -1 | -1 |
| G: -6290.53967 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.02986 HOMO: -6.96884 LUMO: -0.97961 factor:1 | 1 (-0.12449) | -1 | -1 |
| G: -6290.53967 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.99214 HOMO: -6.45998 LUMO: 0.09796 factor:1 | 1 (-0.08678) | -1 | -1 |
| G: -6290.53967 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.32070 HOMO: -6.44638 LUMO: 0.09524 factor:1 | 1 (-0.41533) | -1 | -1 |
| G: -6290.53967 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.17234 HOMO: -6.16338 LUMO: -0.54151 factor:1 | 1 (-0.26697) | -1 | -1 |
| G: -6290.53967 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.45336 HOMO: -6.35930 LUMO: -0.47892 factor:1 | -1 (0.45201) | -1 | -1 |
| G: -6290.53967 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.56604 HOMO: -6.65318 LUMO: -0.00272 factor:1 | -1 (0.33933) | -1 | -1 |
| G: -6290.53967 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.59407 HOMO: -6.50080 LUMO: 0.14694 factor:1 | -1 (0.31130) | -1 | -1 |
| G: -6290.53967 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.70833 HOMO: -6.60420 LUMO: 0.94968 factor:1 | -1 (0.19704) | -1 | -1 |
| G: -6290.53967 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.32947 HOMO: -6.60148 LUMO: -0.77552 factor:1 | -1 (0.57590) | -1 | -1 |
| G: -6290.53967 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.38666 HOMO: -6.81645 LUMO: -1.05580 factor:1 | -1 (0.51870) | -1 | -1 |
| G: -6290.53967 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.43706 HOMO: -6.57971 LUMO: -0.82178 factor:1 | -1 (0.46831) | -1 | -1 |
| G: -6290.53967 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.62566 HOMO: -6.09263 LUMO: -0.45171 factor:1 | -1 (0.27971) | -1 | -1 |
| G: -6290.53967 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.51948 HOMO: -6.74298 LUMO: -0.61770 factor:1 | -1 (0.38588) | -1 | -1 |
| G: -6290.53967 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.48922 HOMO: -6.72393 LUMO: 1.21091 factor:1 | -1 (0.41614) | -1 | -1 |
| G: -6290.53967 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.33834 HOMO: -6.30488 LUMO: 1.70071 factor:1 | -1 (0.56703) | -1 | -1 |
| G: -6290.53967 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.45330 HOMO: -6.38107 LUMO: 1.55649 factor:1 | 1 (-0.54793) | -1 | -1 |
| G: -6290.53967 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.46927 HOMO: -6.17154 LUMO: 1.46669 factor:1 | 1 (-0.56390) | -1 | -1 |
| G: -6290.53967 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.21560 HOMO: -6.86543 LUMO: 1.98643 factor:1 | 1 (-0.31024) | -1 | -1 |
| G: -6290.53967 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.54524 HOMO: -6.69944 LUMO: 1.65173 factor:1 | 1 (-0.63988) | -1 | -1 |
| G: -6290.53967 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.30859 HOMO: -6.77836 LUMO: 2.16331 factor:1 | 1 (-0.40322) | -1 | -1 |
| G: -6290.53967 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.15718 HOMO: -6.42189 LUMO: 2.36467 factor:1 | 1 (-0.25181) | -1 | -1 |
| G: -6290.53967 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.97383 HOMO: -7.00965 LUMO: 2.04358 factor:1 | 1 (-0.06846) | -1 | -1 |
| G: -6290.53967 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.38042 HOMO: -6.36746 LUMO: 2.13881 factor:1 | 1 (-0.47506) | -1 | -1 |
| G: -6290.53967 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.17073 HOMO: -6.37835 LUMO: 1.89935 factor:1 | 1 (-0.26537) | -1 | -1 |
| G: -6290.53967 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.34355 HOMO: -7.03959 LUMO: 1.27349 factor:1 | 1 (-0.43818) | -1 | -1 |
| G: -6290.53967 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.29865 HOMO: -6.67495 LUMO: -0.89253 factor:1 | 1 (-0.39329) | -1 | -1 |
| G: -6290.53967 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.10551 HOMO: -6.71849 LUMO: -0.97961 factor:1 | 1 (-0.20014) | -1 | -1 |
| G: -6290.53967 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.00766 HOMO: -6.47903 LUMO: 0.01633 factor:1 | 1 (-0.10229) | -1 | -1 |
| G: -6290.53967 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.39501 HOMO: -6.38379 LUMO: 0.01088 factor:1 | 1 (-0.48964) | -1 | -1 |
| G: -6290.53967 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.25174 HOMO: -6.49536 LUMO: -0.55239 factor:1 | 1 (-0.34637) | -1 | -1 |
| G: -6290.53967 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.95043 HOMO: -6.53345 LUMO: -0.53879 factor:1 | 1 (-0.04506) | -1 | -1 |
| G: -6290.53967 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.90599 HOMO: -6.16610 LUMO: 2.15514 factor:1 | 1 (-0.00063) | -1 | -1 |
| G: -6290.53967 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.79331 HOMO: -6.35114 LUMO: 1.98643 factor:1 | -1 (0.11206) | -1 | -1 |
| G: -6290.53967 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.46476 HOMO: -6.43277 LUMO: 2.16058 factor:1 | -1 (0.44061) | -1 | -1 |
| G: -6290.53967 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.19547 HOMO: -6.89809 LUMO: 2.20684 factor:1 | 1 (-0.29010) | -1 | -1 |
| G: -6290.53967 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.06020 HOMO: -6.54434 LUMO: 1.93473 factor:1 | 1 (-0.15483) | -1 | -1 |
| G: -6290.53967 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.85639 HOMO: -6.72938 LUMO: 2.03269 factor:1 | -1 (0.04898) | -1 | -1 |
| G: -6290.53967 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.24048 HOMO: -6.90353 LUMO: 2.19868 factor:1 | 1 (-0.33511) | -1 | -1 |
| G: -6290.53967 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.06317 HOMO: -6.41372 LUMO: 2.02453 factor:1 | 1 (-0.15780) | -1 | -1 |
| G: -6290.53967 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.20154 HOMO: -6.46543 LUMO: 1.90752 factor:1 | 1 (-0.29617) | -1 | -1 |
| G: -6290.53967 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.41819 HOMO: -6.55522 LUMO: 2.11977 factor:1 | 1 (-0.51283) | -1 | -1 |
| G: -6290.53967 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.97078 HOMO: -6.28855 LUMO: 2.02181 factor:1 | 1 (-0.06542) | -1 | -1 |
| G: -6290.53967 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.90708 HOMO: -6.45726 LUMO: 1.52112 factor:1 | 1 (-0.00171) | -1 | -1 |
| G: -6290.53967 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.99133 HOMO: -6.37291 LUMO: 2.11705 factor:1 | 1 (-0.08596) | -1 | -1 |
| G: -6290.53967 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.35686 HOMO: -6.88448 LUMO: 2.24494 factor:1 | 1 (-0.45149) | -1 | -1 |
| G: -6290.53967 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.15615 HOMO: -6.86271 LUMO: 2.41637 factor:1 | 1 (-0.25078) | -1 | -1 |
| G: -6290.53967 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.22790 HOMO: -6.69400 LUMO: 2.34562 factor:1 | 1 (-0.32254) | -1 | -1 |
| G: -6290.53967 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.13960 HOMO: -6.18243 LUMO: 2.53882 factor:1 | 1 (-0.23424) | -1 | -1 |
| G: -6290.53967 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.36355 HOMO: -6.61237 LUMO: 2.54154 factor:1 | 1 (-0.45819) | -1 | -1 |
| G: -6290.53967 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.86058 HOMO: -6.69672 LUMO: 2.16331 factor:1 | -1 (0.04479) | -1 | -1 |
| G: -6290.53967 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.73361 HOMO: -6.33481 LUMO: 2.34018 factor:1 | -1 (0.17176) | -1 | -1 |
| G: -6290.53967 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.83489 HOMO: -5.99739 LUMO: 2.37283 factor:1 | -1 (0.07048) | -1 | -1 |
| G: -6290.53967 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.46999 HOMO: -6.49808 LUMO: 2.47351 factor:1 | -1 (0.43538) | -1 | -1 |
| G: -6290.53967 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.11628 HOMO: -6.22052 LUMO: 1.86398 factor:1 | 1 (-0.21092) | -1 | -1 |
| G: -6290.53967 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.91271 HOMO: -6.32665 LUMO: 2.28031 factor:1 | 1 (-0.00735) | -1 | -1 |
| G: -6290.53967 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.90833 HOMO: -5.98378 LUMO: 2.16331 factor:1 | 1 (-0.00297) | -1 | -1 |
| G: -6290.53967 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.82675 HOMO: -6.08991 LUMO: 2.30208 factor:1 | -1 (0.07861) | -1 | -1 |
| G: -6290.53967 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.64019 HOMO: -7.07224 LUMO: 1.55105 factor:1 | -1 (0.26517) | 1 | 1 |
| G: -6290.53967 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.11182 HOMO: -6.84638 LUMO: 1.76874 factor:1 | 1 (-0.20645) | -1 | -1 |
| G: -6290.53967 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.80557 HOMO: -6.68856 LUMO: 1.47758 factor:1 | 1 (-0.90021) | -1 | -1 |
| G: -6290.53967 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12556.58268 HOMO: -6.69672 LUMO: 1.71976 factor:1 | 1 (-1.67731) | -1 | -1 |
| G: -6290.53967 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.45983 HOMO: -6.86543 LUMO: 2.24766 factor:1 | 1 (-0.55446) | -1 | -1 |
| G: -6290.53967 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.60160 HOMO: -7.21646 LUMO: 1.71976 factor:1 | 1 (-0.69623) | 1 | 1 |
| G: -6290.53967 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.80664 HOMO: -6.94162 LUMO: 2.21773 factor:1 | 1 (-0.90127) | -1 | -1 |
| G: -6290.53967 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.39713 HOMO: -6.34842 LUMO: 2.04358 factor:1 | 1 (-0.49176) | -1 | -1 |
| G: -6290.53967 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.89643 HOMO: -6.53345 LUMO: 1.96738 factor:1 | 1 (-0.99107) | -1 | -1 |
| G: -6290.53967 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12556.40423 HOMO: -6.34842 LUMO: 1.88303 factor:1 | 1 (-1.49886) | -1 | -1 |
| G: -6290.53967 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12556.12193 HOMO: -6.38651 LUMO: 2.08983 factor:1 | 1 (-1.21657) | -1 | -1 |
| G: -6290.53967 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12556.58015 HOMO: -6.01372 LUMO: 1.43676 factor:1 | 1 (-1.67478) | -1 | -1 |
| G: -6290.53967 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.42173 HOMO: -6.30216 LUMO: 1.41771 factor:1 | 1 (-0.51636) | -1 | -1 |
| G: -6290.53967 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.23816 HOMO: -6.52801 LUMO: 1.77146 factor:1 | 1 (-0.33280) | -1 | -1 |
| G: -6290.53967 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.05566 HOMO: -6.53617 LUMO: 1.72792 factor:1 | 1 (-0.15029) | -1 | -1 |
| G: -6290.53967 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12556.52153 HOMO: -6.56611 LUMO: 2.20412 factor:1 | 1 (-1.61617) | -1 | -1 |
| G: -6290.53967 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.73961 HOMO: -6.66679 LUMO: -0.72927 factor:1 | 1 (-0.83425) | -1 | -1 |
| G: -6290.53967 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12556.66714 HOMO: -6.85455 LUMO: -0.85444 factor:1 | 1 (-1.76177) | -1 | -1 |
| G: -6290.53967 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.36274 HOMO: -7.21646 LUMO: 0.27211 factor:1 | 1 (-0.45737) | 1 | 1 |
| G: -6290.53967 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12556.13257 HOMO: -6.57971 LUMO: -0.41361 factor:1 | 1 (-1.22721) | -1 | -1 |
| G: -6290.53967 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.88773 HOMO: -7.03142 LUMO: -1.14288 factor:1 | 1 (-0.98236) | -1 | -1 |
| G: -6290.53967 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.67365 HOMO: -6.29944 LUMO: 0.06803 factor:1 | 1 (-0.76829) | -1 | -1 |
| G: -6290.53967 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.52623 HOMO: -6.47359 LUMO: 0.28028 factor:1 | -1 (0.37914) | -1 | -1 |
| G: -6290.53967 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.39515 HOMO: -6.42189 LUMO: 1.61364 factor:1 | -1 (0.51021) | -1 | -1 |
| G: -6290.53967 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.93986 HOMO: -6.41100 LUMO: 1.80956 factor:1 | 1 (-1.03450) | -1 | -1 |
| G: -6290.53967 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.39808 HOMO: -6.83278 LUMO: 1.83949 factor:1 | 1 (-0.49272) | -1 | -1 |
| G: -6290.53967 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.79034 HOMO: -6.78380 LUMO: -0.76192 factor:1 | 1 (-0.88497) | -1 | -1 |
| G: -6290.53967 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.34219 HOMO: -6.95795 LUMO: 2.13609 factor:1 | 1 (-0.43682) | -1 | -1 |
| G: -6290.53967 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.28611 HOMO: -6.57155 LUMO: 1.89119 factor:1 | 1 (-0.38074) | -1 | -1 |
| G: -6290.53967 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.39599 HOMO: -6.65591 LUMO: 1.93745 factor:1 | 1 (-0.49062) | -1 | -1 |
| G: -6290.53967 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.31789 HOMO: -6.44638 LUMO: 2.26943 factor:1 | 1 (-0.41252) | -1 | -1 |
| G: -6290.53967 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.45928 HOMO: -5.88038 LUMO: 1.90480 factor:1 | 1 (-0.55391) | -1 | -1 |
| G: -6290.53967 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.24505 HOMO: -6.22052 LUMO: 2.17691 factor:1 | 1 (-0.33968) | -1 | -1 |
| G: -6290.53967 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.11258 HOMO: -6.04637 LUMO: 2.23950 factor:1 | 1 (-0.20721) | -1 | -1 |
| G: -6290.53967 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.18151 HOMO: -6.44366 LUMO: 2.24766 factor:1 | 1 (-0.27614) | -1 | -1 |
| G: -6290.53967 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.89111 HOMO: -6.81917 LUMO: 2.08439 factor:1 | -1 (0.01426) | -1 | -1 |
| G: -6290.53967 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.63368 HOMO: -6.48447 LUMO: 2.28576 factor:1 | 1 (-0.72831) | -1 | -1 |
| G: -6290.53967 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.82449 HOMO: -6.54434 LUMO: 1.99187 factor:1 | 1 (-0.91912) | -1 | -1 |
| G: -6290.53967 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.62680 HOMO: -6.17698 LUMO: -0.65852 factor:1 | 1 (-0.72143) | -1 | -1 |
| G: -6290.53967 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.85341 HOMO: -6.08174 LUMO: -0.58504 factor:1 | 1 (-0.94804) | -1 | -1 |
| G: -6290.53967 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12556.43340 HOMO: -6.55250 LUMO: -0.86804 factor:1 | 1 (-1.52803) | -1 | -1 |
| G: -6290.53967 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.65975 HOMO: -6.57699 LUMO: -0.89525 factor:1 | 1 (-0.75438) | -1 | -1 |
| G: -6290.53967 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12556.13021 HOMO: -6.63141 LUMO: -1.04220 factor:1 | 1 (-1.22484) | -1 | -1 |
| G: -6290.53967 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12556.21704 HOMO: -6.69128 LUMO: -0.76736 factor:1 | 1 (-1.31167) | -1 | -1 |
| G: -6290.53967 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.49700 HOMO: -6.25318 LUMO: -1.03131 factor:1 | 1 (-0.59163) | -1 | -1 |
| G: -6290.53967 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12556.06212 HOMO: -6.69944 LUMO: 0.01905 factor:1 | 1 (-1.15676) | -1 | -1 |
| G: -6290.53967 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.34369 HOMO: -6.28583 LUMO: 0.38368 factor:1 | 1 (-0.43832) | -1 | -1 |
| G: -6290.53967 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.41808 HOMO: -6.90081 LUMO: -0.83811 factor:1 | 1 (-0.51272) | -1 | -1 |
| G: -6290.53967 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.62152 HOMO: -6.78380 LUMO: -0.10068 factor:1 | 1 (-0.71615) | -1 | -1 |
| G: -6290.53967 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.46562 HOMO: -6.30488 LUMO: -0.98505 factor:1 | 1 (-0.56026) | -1 | -1 |
| G: -6290.53967 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.23713 HOMO: -6.29671 LUMO: -1.79051 factor:1 | 1 (-0.33176) | -1 | -1 |
| G: -6290.53967 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.25264 HOMO: -6.76747 LUMO: -0.22041 factor:1 | 1 (-0.34727) | -1 | -1 |
| G: -6290.53967 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.60455 HOMO: -6.22597 LUMO: -0.94968 factor:1 | -1 (0.30082) | -1 | -1 |
| G: -6290.53967 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.38381 HOMO: -6.73482 LUMO: 0.05987 factor:1 | -1 (0.52156) | -1 | -1 |
| G: -6290.53967 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.30209 HOMO: -6.28855 LUMO: 0.34831 factor:1 | -1 (0.60328) | -1 | -1 |
| G: -6290.53967 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.56188 HOMO: -6.69400 LUMO: 0.25307 factor:1 | -1 (0.34349) | -1 | -1 |
| G: -6290.53967 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.51208 HOMO: -6.70216 LUMO: 0.61226 factor:1 | -1 (0.39329) | -1 | -1 |
| G: -6290.53967 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.11390 HOMO: -6.70216 LUMO: 0.17415 factor:1 | -1 (0.79147) | -1 | -1 |
| G: -6290.53967 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.38879 HOMO: -6.70761 LUMO: 0.24762 factor:1 | -1 (0.51658) | -1 | -1 |
| G: -6290.53967 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.31853 HOMO: -6.68856 LUMO: -0.84900 factor:1 | -1 (0.58684) | -1 | -1 |
| G: -6290.53967 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.34990 HOMO: -6.71033 LUMO: -0.38640 factor:1 | -1 (0.55547) | -1 | -1 |
| G: -6290.53967 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.18759 HOMO: -6.24501 LUMO: -0.09252 factor:1 | -1 (0.71778) | -1 | -1 |
| G: -6290.53967 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.54659 HOMO: -6.81645 LUMO: -0.07347 factor:1 | -1 (0.35878) | -1 | -1 |
| G: -6290.53967 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.32462 HOMO: -6.49536 LUMO: 0.09796 factor:1 | -1 (0.58075) | -1 | -1 |
| G: -6290.53967 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.71787 HOMO: -6.71033 LUMO: -0.26395 factor:1 | 1 (-0.81250) | -1 | -1 |
| G: -6290.53967 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12556.50834 HOMO: -6.70489 LUMO: -0.09252 factor:1 | 1 (-1.60297) | -1 | -1 |
| G: -6290.53967 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12556.25900 HOMO: -6.23685 LUMO: 0.39729 factor:1 | 1 (-1.35363) | -1 | -1 |
| G: -6290.53967 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.60573 HOMO: -6.69400 LUMO: -0.05442 factor:1 | 1 (-0.70037) | -1 | -1 |
| G: -6290.53967 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.16707 HOMO: -6.36202 LUMO: 0.09796 factor:1 | -1 (0.73830) | -1 | -1 |
| G: -6290.53967 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.39722 HOMO: -6.54978 LUMO: 0.15510 factor:1 | -1 (0.50815) | -1 | -1 |
| G: -6290.53967 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.86778 HOMO: -6.77836 LUMO: 0.25851 factor:1 | 1 (-0.96241) | -1 | -1 |
| G: -6290.53967 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.19786 HOMO: -5.70623 LUMO: 0.73471 factor:1 | 1 (-0.29250) | -1 | -1 |
| G: -6290.53967 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12556.00384 HOMO: -5.58378 LUMO: 0.89253 factor:1 | 1 (-1.09847) | -1 | -1 |
| G: -6290.53967 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.90718 HOMO: -5.68718 LUMO: 0.87893 factor:1 | 1 (-1.00181) | -1 | -1 |
| G: -6290.53967 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.69028 HOMO: -5.10486 LUMO: 1.11567 factor:1 | 1 (-0.78491) | -1 | -1 |
| G: -6290.53967 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.97155 HOMO: -4.59328 LUMO: 1.27621 factor:1 | 1 (-0.06618) | -1 | -1 |
| G: -6290.53967 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.27920 HOMO: -4.45450 LUMO: 1.82044 factor:1 | 1 (-0.37383) | -1 | -1 |
| G: -6290.53967 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.40753 HOMO: -4.64226 LUMO: 1.70615 factor:1 | 1 (-0.50216) | -1 | -1 |
| G: -6290.53967 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.37204 HOMO: -5.04227 LUMO: 1.04492 factor:1 | 1 (-0.46668) | -1 | -1 |
| G: -6290.53967 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.35400 HOMO: -4.85723 LUMO: 0.93607 factor:1 | 1 (-0.44863) | -1 | -1 |
| G: -6290.53967 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.26965 HOMO: -4.72934 LUMO: 1.00410 factor:1 | 1 (-0.36428) | -1 | -1 |
| G: -6290.53967 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.56494 HOMO: -4.56335 LUMO: 1.56738 factor:1 | 1 (-0.65958) | -1 | -1 |
| G: -6290.53967 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.58816 HOMO: -5.48854 LUMO: 0.33198 factor:1 | 1 (-0.68279) | -1 | -1 |
| G: -6290.53967 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.36513 HOMO: -4.97424 LUMO: 1.33608 factor:1 | 1 (-0.45976) | -1 | -1 |
| G: -6290.53967 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.40862 HOMO: -4.60145 LUMO: 1.74697 factor:1 | 1 (-0.50325) | -1 | -1 |
| G: -6290.53967 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.10551 HOMO: -5.60010 LUMO: 0.74831 factor:1 | 1 (-0.20014) | -1 | -1 |
| G: -6290.53967 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.22761 HOMO: -5.66541 LUMO: 0.66668 factor:1 | -1 (0.67775) | -1 | -1 |
| G: -6290.53967 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.08201 HOMO: -6.50080 LUMO: 0.07075 factor:1 | -1 (0.82336) | -1 | -1 |
| G: -6290.53967 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.09991 HOMO: -5.79603 LUMO: 0.22313 factor:1 | -1 (0.80546) | -1 | -1 |
| G: -6290.53967 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12553.83993 HOMO: -4.68036 LUMO: 1.29798 factor:1 | -1 (1.06543) | -1 | -1 |
| G: -6290.53967 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.28459 HOMO: -4.84363 LUMO: 1.34424 factor:1 | -1 (0.62077) | -1 | -1 |
| G: -6290.53967 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.99962 HOMO: -4.62321 LUMO: 1.82861 factor:1 | 1 (-1.09425) | -1 | -1 |
| G: -6290.53967 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.73978 HOMO: -5.83684 LUMO: 0.82178 factor:1 | 1 (-0.83441) | -1 | -1 |
| G: -6290.53967 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12556.05709 HOMO: -5.27629 LUMO: 0.57960 factor:1 | 1 (-1.15172) | -1 | -1 |
| G: -6290.53967 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.32848 HOMO: -5.15928 LUMO: -2.96876 factor:1 | 1 (-0.42311) | -1 | -1 |
| G: -6290.53967 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.05522 HOMO: -5.08853 LUMO: 0.89253 factor:1 | 1 (-0.14985) | -1 | -1 |
| G: -6290.53967 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.89976 HOMO: -6.42461 LUMO: 0.04354 factor:1 | -1 (0.00561) | -1 | -1 |
| G: -6290.53967 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.09280 HOMO: -6.42733 LUMO: -0.00544 factor:1 | 1 (-0.18743) | -1 | -1 |
| G: -6290.53967 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.24516 HOMO: -5.87494 LUMO: 0.69933 factor:1 | 1 (-0.33979) | -1 | -1 |
| G: -6290.53967 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.22695 HOMO: -5.07492 LUMO: 1.02587 factor:1 | 1 (-0.32158) | -1 | -1 |
| G: -6290.53967 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.92885 HOMO: -4.44362 LUMO: 1.99187 factor:1 | 1 (-0.02348) | -1 | -1 |
| G: -6290.53967 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.04507 HOMO: -5.82052 LUMO: 0.43810 factor:1 | 1 (-0.13970) | -1 | -1 |
| G: -6290.53967 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.79405 HOMO: -5.75793 LUMO: 0.76464 factor:1 | -1 (0.11132) | -1 | -1 |
| G: -6290.53967 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.23476 HOMO: -5.09669 LUMO: 0.72382 factor:1 | 1 (-0.32939) | -1 | -1 |
| G: -6290.53967 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.38944 HOMO: -6.75387 LUMO: -2.02453 factor:1 | -1 (0.51593) | -1 | -1 |
| G: -6290.53967 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.58509 HOMO: -5.02322 LUMO: 1.14832 factor:1 | -1 (0.32028) | -1 | -1 |
| G: -6290.53967 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.52014 HOMO: -5.75521 LUMO: 0.73471 factor:1 | -1 (0.38523) | -1 | -1 |
| G: -6290.53967 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.48637 HOMO: -5.89943 LUMO: 0.54967 factor:1 | -1 (0.41900) | -1 | -1 |
| G: -6290.53967 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.19240 HOMO: -5.80147 LUMO: 0.72382 factor:1 | -1 (0.71297) | -1 | -1 |
| G: -6290.53967 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.33186 HOMO: -6.16066 LUMO: 0.39457 factor:1 | -1 (0.57351) | -1 | -1 |
| G: -6290.53967 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.55497 HOMO: -5.98650 LUMO: 0.76736 factor:1 | -1 (0.35040) | -1 | -1 |
| G: -6290.53967 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.78414 HOMO: -4.74839 LUMO: 1.88847 factor:1 | -1 (0.12123) | -1 | -1 |
| G: -6290.53967 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.75535 HOMO: -5.62459 LUMO: 0.26939 factor:1 | -1 (0.15002) | -1 | -1 |
| G: -6290.53967 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.48022 HOMO: -4.88172 LUMO: 1.30070 factor:1 | -1 (0.42515) | -1 | -1 |
| G: -6290.53967 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.55739 HOMO: -5.09397 LUMO: 0.98505 factor:1 | -1 (0.34798) | -1 | -1 |
| G: -6290.53967 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.23123 HOMO: -6.50080 LUMO: -0.28300 factor:1 | -1 (0.67413) | -1 | -1 |
| G: -6290.53967 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.33513 HOMO: -5.04227 LUMO: 1.49935 factor:1 | -1 (0.57024) | -1 | -1 |
| G: -6290.53967 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.20522 HOMO: -5.22731 LUMO: 0.88437 factor:1 | -1 (0.70015) | -1 | -1 |
| G: -6290.53967 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.04503 HOMO: -4.95519 LUMO: 1.25717 factor:1 | -1 (0.86034) | -1 | -1 |
| G: -6290.53967 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.33567 HOMO: -4.61233 LUMO: 1.27621 factor:1 | -1 (0.56970) | -1 | -1 |
| G: -6290.53967 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.57415 HOMO: -4.70757 LUMO: 1.63813 factor:1 | -1 (0.33122) | -1 | -1 |
| G: -6290.53967 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.62776 HOMO: -4.85179 LUMO: 1.11839 factor:1 | -1 (0.27761) | -1 | -1 |
| G: -6290.53967 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.35330 HOMO: -4.97696 LUMO: 1.00138 factor:1 | -1 (0.55206) | -1 | -1 |
| G: -6290.53967 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.57284 HOMO: -5.64636 LUMO: 0.81090 factor:1 | -1 (0.33252) | -1 | -1 |
| G: -6290.53967 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.47042 HOMO: -4.37831 LUMO: 1.90208 factor:1 | -1 (0.43495) | -1 | -1 |
| G: -6290.53967 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.67026 HOMO: -4.67764 LUMO: 1.54561 factor:1 | -1 (0.23511) | -1 | -1 |
| G: -6290.53967 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.17052 HOMO: -5.87766 LUMO: 0.42994 factor:1 | 1 (-0.26515) | -1 | -1 |
| G: -6290.53967 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.33591 HOMO: -6.03821 LUMO: 0.32382 factor:1 | 1 (-0.43054) | -1 | -1 |
| G: -6290.53967 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.04330 HOMO: -5.99739 LUMO: 0.69389 factor:1 | 1 (-0.13793) | -1 | -1 |
| G: -6290.53967 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.11054 HOMO: -6.43821 LUMO: 0.15238 factor:1 | 1 (-0.20517) | -1 | -1 |
| G: -6290.53967 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.02442 HOMO: -6.63414 LUMO: -0.07347 factor:1 | 1 (-0.11905) | -1 | -1 |
| G: -6290.53967 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.08181 HOMO: -6.50080 LUMO: 0.10068 factor:1 | 1 (-0.17644) | -1 | -1 |
| G: -6290.53967 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.56985 HOMO: -6.49264 LUMO: 0.19592 factor:1 | -1 (0.33552) | -1 | -1 |
| G: -6290.53967 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.31379 HOMO: -5.83956 LUMO: 0.12517 factor:1 | -1 (0.59158) | -1 | -1 |
| G: -6290.53967 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.13295 HOMO: -6.50896 LUMO: 0.19048 factor:1 | -1 (0.77242) | -1 | -1 |
| G: -6290.53967 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12553.95498 HOMO: -6.56611 LUMO: 0.04898 factor:1 | -1 (0.95038) | -1 | -1 |
| G: -6290.53967 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.25401 HOMO: -6.68040 LUMO: -0.08436 factor:1 | -1 (0.65136) | -1 | -1 |
| G: -6290.53967 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.38432 HOMO: -6.73754 LUMO: -0.08708 factor:1 | -1 (0.52104) | -1 | -1 |
| G: -6290.53967 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.34198 HOMO: -6.80285 LUMO: -0.10612 factor:1 | -1 (0.56338) | -1 | -1 |
| G: -6290.53967 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.29774 HOMO: -6.35658 LUMO: 0.02177 factor:1 | -1 (0.60763) | -1 | -1 |
| G: -6290.53967 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.05771 HOMO: -5.74160 LUMO: 0.14694 factor:1 | -1 (0.84766) | -1 | -1 |
| G: -6290.53967 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.25414 HOMO: -4.78376 LUMO: 0.92791 factor:1 | -1 (0.65122) | -1 | -1 |
| G: -6290.53967 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.15757 HOMO: -5.90215 LUMO: 0.36463 factor:1 | -1 (0.74780) | -1 | -1 |
| G: -6290.53967 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12553.84864 HOMO: -4.99329 LUMO: 0.85988 factor:1 | -1 (1.05673) | -1 | -1 |
| G: -6290.53967 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.50375 HOMO: -4.93887 LUMO: 1.33608 factor:1 | -1 (0.40161) | -1 | -1 |
| G: -6290.53967 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.16968 HOMO: -5.19193 LUMO: 0.50341 factor:1 | -1 (0.73569) | -1 | -1 |
| G: -6290.53967 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.49959 HOMO: -6.64502 LUMO: -1.98643 factor:1 | -1 (0.40578) | -1 | -1 |
| G: -6290.53967 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.33608 HOMO: -5.15384 LUMO: 0.94968 factor:1 | -1 (0.56929) | -1 | -1 |
| G: -6290.53967 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.13009 HOMO: -6.31032 LUMO: 0.08436 factor:1 | -1 (0.77528) | -1 | -1 |
| G: -6290.53967 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12553.82959 HOMO: -4.88716 LUMO: 0.82995 factor:1 | -1 (1.07577) | -1 | -1 |
| G: -6290.53967 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.32528 HOMO: -5.57017 LUMO: 0.19320 factor:1 | -1 (0.58009) | -1 | -1 |
| G: -6290.53967 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.51233 HOMO: -4.92254 LUMO: 0.93879 factor:1 | -1 (0.39304) | -1 | -1 |
| G: -6290.53967 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.45235 HOMO: -4.77288 LUMO: 1.60003 factor:1 | -1 (0.45302) | -1 | -1 |
| G: -6290.53967 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.26253 HOMO: -4.97696 LUMO: 0.89798 factor:1 | -1 (0.64284) | -1 | -1 |
| G: -6290.53967 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.26508 HOMO: -5.00690 LUMO: 1.14288 factor:1 | -1 (0.64028) | -1 | -1 |
| G: -6290.53967 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12553.90959 HOMO: -4.88444 LUMO: 1.48574 factor:1 | -1 (0.99577) | -1 | -1 |
| G: -6290.53967 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.08103 HOMO: -5.03955 LUMO: 1.51023 factor:1 | -1 (0.82434) | -1 | -1 |
| G: -6290.53967 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.10432 HOMO: -5.22459 LUMO: 0.99049 factor:1 | -1 (0.80105) | -1 | -1 |
| G: -6290.53967 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12553.83237 HOMO: -5.29534 LUMO: 0.96056 factor:1 | -1 (1.07300) | -1 | -1 |
| G: -6290.53967 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.36974 HOMO: -5.35520 LUMO: 0.68301 factor:1 | -1 (0.53563) | -1 | -1 |
| G: -6290.53967 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.66830 HOMO: -5.27357 LUMO: 1.18642 factor:1 | -1 (0.23707) | -1 | -1 |
| G: -6290.53967 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.43494 HOMO: -5.79875 LUMO: 0.61770 factor:1 | -1 (0.47043) | -1 | -1 |
| G: -6290.53967 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.58071 HOMO: -7.64640 LUMO: -2.45175 factor:1 | -1 (0.32466) | -1 | -1 |
| G: -6290.53967 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.66626 HOMO: -7.46953 LUMO: -1.29798 factor:1 | -1 (0.23911) | 1 | 1 |
| G: -6290.53967 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.72863 HOMO: -7.95389 LUMO: -0.37280 factor:1 | -1 (0.17674) | 1 | 1 |
| G: -6290.53967 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.43926 HOMO: -7.23279 LUMO: -1.19186 factor:1 | -1 (0.46610) | 1 | 1 |
| G: -6290.53967 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.39200 HOMO: -7.14299 LUMO: -1.12927 factor:1 | -1 (0.51337) | 1 | 1 |
| G: -6290.53967 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.64134 HOMO: -6.93074 LUMO: 0.31565 factor:1 | -1 (0.26403) | -1 | -1 |
| G: -6290.53967 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.34030 HOMO: -6.63141 LUMO: 0.28028 factor:1 | -1 (0.56507) | -1 | -1 |
| G: -6290.53967 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.58479 HOMO: -7.10489 LUMO: -1.07213 factor:1 | -1 (0.32058) | 1 | 1 |
| G: -6290.53967 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.62939 HOMO: -7.00693 LUMO: -0.69389 factor:1 | -1 (0.27598) | -1 | -1 |
| G: -6290.53967 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.41983 HOMO: -8.50356 LUMO: -1.79595 factor:1 | -1 (0.48553) | -1 | -1 |
| G: -6290.53967 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.28323 HOMO: -7.79334 LUMO: -2.33746 factor:1 | -1 (0.62213) | -1 | -1 |
| G: -6290.53967 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.36514 HOMO: -7.24367 LUMO: -0.85172 factor:1 | -1 (0.54023) | 1 | 1 |
| G: -6290.53967 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.48258 HOMO: -7.94028 LUMO: -0.20136 factor:1 | -1 (0.42278) | 1 | 1 |
| G: -6290.53967 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.52792 HOMO: -7.22462 LUMO: 0.84627 factor:1 | -1 (0.37745) | 1 | 1 |
| G: -6290.53967 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.32729 HOMO: -6.54978 LUMO: 0.34831 factor:1 | -1 (0.57808) | -1 | -1 |
| G: -6290.53967 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.14002 HOMO: -6.86815 LUMO: 0.32109 factor:1 | -1 (0.76535) | -1 | -1 |
| G: -6290.53967 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12553.86426 HOMO: -7.17564 LUMO: -1.28438 factor:1 | -1 (1.04111) | 1 | 1 |
| G: -6290.53967 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.39219 HOMO: -7.03142 LUMO: -1.12655 factor:1 | -1 (0.51318) | -1 | -1 |
| G: -6290.53967 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.37025 HOMO: -7.39878 LUMO: 0.15783 factor:1 | 1 (-0.46488) | 1 | 1 |
| G: -6290.53967 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.39411 HOMO: -7.25728 LUMO: 0.42178 factor:1 | 1 (-0.48874) | 1 | 1 |
| G: -6290.53967 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.37863 HOMO: -6.86543 LUMO: 0.93879 factor:1 | 1 (-0.47326) | -1 | -1 |
| G: -6290.53967 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.95620 HOMO: -7.09673 LUMO: -0.69661 factor:1 | 1 (-0.05083) | 1 | 1 |
| G: -6290.53967 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.18173 HOMO: -7.74708 LUMO: 0.01088 factor:1 | 1 (-0.27636) | 1 | 1 |
| G: -6290.53967 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.09231 HOMO: -6.80557 LUMO: 0.46531 factor:1 | 1 (-0.18694) | -1 | -1 |
| G: -6290.53967 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.16377 HOMO: -7.29265 LUMO: 1.31975 factor:1 | 1 (-0.25840) | 1 | 1 |
| G: -6290.53967 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.60196 HOMO: -6.93618 LUMO: 0.29388 factor:1 | -1 (0.30341) | -1 | -1 |
| G: -6290.53967 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.35189 HOMO: -6.53073 LUMO: 0.71022 factor:1 | -1 (0.55348) | -1 | -1 |
| G: -6290.53967 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.38612 HOMO: -6.41917 LUMO: -1.24084 factor:1 | -1 (0.51925) | -1 | -1 |
| G: -6290.53967 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.20595 HOMO: -6.67495 LUMO: -1.09118 factor:1 | -1 (0.69941) | -1 | -1 |
| G: -6290.53967 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.16097 HOMO: -6.97156 LUMO: -0.53606 factor:1 | -1 (0.74439) | -1 | -1 |
| G: -6290.53967 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.10116 HOMO: -6.85183 LUMO: -0.45715 factor:1 | -1 (0.80421) | -1 | -1 |
| G: -6290.53967 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12553.93531 HOMO: -7.12666 LUMO: -0.67484 factor:1 | -1 (0.97006) | 1 | 1 |
| G: -6290.53967 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.35110 HOMO: -7.49946 LUMO: -0.14694 factor:1 | -1 (0.55427) | 1 | 1 |
| G: -6290.53967 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.32440 HOMO: -7.44231 LUMO: 0.58232 factor:1 | -1 (0.58096) | 1 | 1 |
| G: -6290.53967 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.20744 HOMO: -7.36340 LUMO: -0.68301 factor:1 | 1 (-0.30207) | 1 | 1 |
| G: -6290.53967 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.05487 HOMO: -6.13073 LUMO: -0.54967 factor:1 | 1 (-0.14950) | -1 | -1 |
| G: -6290.53967 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.49463 HOMO: -7.81511 LUMO: -0.06531 factor:1 | 1 (-0.58926) | 1 | 1 |
| G: -6290.53967 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.84360 HOMO: -7.26816 LUMO: -1.02587 factor:1 | -1 (0.06177) | 1 | 1 |
| G: -6290.53967 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.88308 HOMO: -7.98110 LUMO: -0.17960 factor:1 | -1 (0.02229) | 1 | 1 |
| G: -6290.53967 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.97971 HOMO: -7.44776 LUMO: -1.00954 factor:1 | 1 (-0.07434) | 1 | 1 |
| G: -6290.53967 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.00752 HOMO: -7.47769 LUMO: -1.02859 factor:1 | 1 (-0.10215) | 1 | 1 |
| G: -6290.53967 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.14012 HOMO: -6.75659 LUMO: 0.39457 factor:1 | 1 (-0.23475) | -1 | -1 |
| G: -6290.53967 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.13383 HOMO: -6.71849 LUMO: 0.36735 factor:1 | 1 (-0.22847) | -1 | -1 |
| G: -6290.53967 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.04123 HOMO: -7.64096 LUMO: -1.43948 factor:1 | 1 (-0.13587) | 1 | 1 |
| G: -6290.53967 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.98518 HOMO: -7.83144 LUMO: -1.36601 factor:1 | 1 (-0.07981) | 1 | 1 |
| G: -6290.53967 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.75995 HOMO: -7.19469 LUMO: 0.35103 factor:1 | -1 (0.14542) | 1 | 1 |
| G: -6290.53967 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.87633 HOMO: -7.03414 LUMO: 0.20409 factor:1 | -1 (0.02903) | -1 | -1 |
| G: -6290.53967 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.93152 HOMO: -7.22734 LUMO: 0.31293 factor:1 | 1 (-0.02615) | 1 | 1 |
| G: -6290.53967 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.22355 HOMO: -6.93618 LUMO: 0.56055 factor:1 | 1 (-0.31818) | -1 | -1 |
| G: -6290.53967 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.00306 HOMO: -6.94707 LUMO: -0.88709 factor:1 | 1 (-0.09769) | -1 | -1 |
| G: -6290.53967 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.05166 HOMO: -6.86543 LUMO: -0.83267 factor:1 | 1 (-0.14629) | -1 | -1 |
| G: -6290.53967 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.29898 HOMO: -6.82189 LUMO: -1.15376 factor:1 | 1 (-0.39361) | -1 | -1 |
| G: -6290.53967 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12556.42110 HOMO: -6.65046 LUMO: -0.46531 factor:1 | 1 (-1.51573) | -1 | -1 |
| G: -6290.53967 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.79624 HOMO: -6.52529 LUMO: 0.20953 factor:1 | 1 (-0.89087) | -1 | -1 |
| G: -6290.53967 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12556.57737 HOMO: -6.80557 LUMO: 0.44355 factor:1 | 1 (-1.67200) | -1 | -1 |
| G: -6290.53967 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.59235 HOMO: -6.93074 LUMO: -0.81634 factor:1 | 1 (-0.68698) | -1 | -1 |
| G: -6290.53967 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.61006 HOMO: -7.43143 LUMO: -0.45987 factor:1 | 1 (-0.70469) | 1 | 1 |
| G: -6290.53967 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12556.43644 HOMO: -7.07224 LUMO: -0.68028 factor:1 | 1 (-1.53108) | 1 | 1 |
| G: -6290.53967 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12556.39827 HOMO: -6.68040 LUMO: -0.71566 factor:1 | 1 (-1.49290) | -1 | -1 |
| G: -6290.53967 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12556.01633 HOMO: -6.26406 LUMO: -1.09934 factor:1 | 1 (-1.11096) | -1 | -1 |
| G: -6290.53967 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12556.39759 HOMO: -5.94569 LUMO: -0.72110 factor:1 | 1 (-1.49222) | -1 | -1 |
| G: -6290.53967 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12556.20077 HOMO: -6.12256 LUMO: -0.42178 factor:1 | 1 (-1.29540) | -1 | -1 |
| G: -6290.53967 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.41242 HOMO: -6.09807 LUMO: 0.11429 factor:1 | 1 (-0.50706) | -1 | -1 |
| G: -6290.53967 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.98346 HOMO: -7.35252 LUMO: -0.55783 factor:1 | 1 (-0.07810) | 1 | 1 |
| G: -6290.53967 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12556.16076 HOMO: -7.57837 LUMO: -0.76736 factor:1 | 1 (-1.25540) | 1 | 1 |
| G: -6290.53967 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.26867 HOMO: -6.16066 LUMO: 0.01905 factor:1 | 1 (-0.36330) | -1 | -1 |
| G: -6290.53967 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.42004 HOMO: -6.13345 LUMO: -0.41906 factor:1 | 1 (-0.51468) | -1 | -1 |
| G: -6290.53967 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.04847 HOMO: -6.10351 LUMO: -0.33742 factor:1 | 1 (-0.14310) | -1 | -1 |
| G: -6290.53967 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.61213 HOMO: -7.24639 LUMO: -0.51702 factor:1 | 1 (-0.70676) | 1 | 1 |
| G: -6290.53967 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.33278 HOMO: -6.98244 LUMO: -1.82044 factor:1 | 1 (-0.42741) | -1 | -1 |
| G: -6290.53967 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.43545 HOMO: -6.37563 LUMO: -1.67622 factor:1 | 1 (-0.53008) | -1 | -1 |
| G: -6290.53967 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.48143 HOMO: -5.79058 LUMO: -2.55243 factor:1 | 1 (-0.57607) | -1 | -1 |
| G: -6290.53967 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.35574 HOMO: -6.34025 LUMO: -0.27483 factor:1 | 1 (-0.45038) | -1 | -1 |
| G: -6290.53967 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.79926 HOMO: -6.05453 LUMO: -0.51157 factor:1 | 1 (-0.89389) | -1 | -1 |
| G: -6290.53967 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.60688 HOMO: -7.53755 LUMO: -0.38912 factor:1 | 1 (-0.70151) | 1 | 1 |
| G: -6290.53967 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.64473 HOMO: -7.00421 LUMO: -0.50885 factor:1 | 1 (-0.73936) | -1 | -1 |
| G: -6290.53967 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.61575 HOMO: -7.52123 LUMO: -0.37552 factor:1 | 1 (-0.71038) | 1 | 1 |
| G: -6290.53967 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.23956 HOMO: -6.70489 LUMO: -1.04764 factor:1 | -1 (0.66581) | -1 | -1 |
| G: -6290.53967 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.40013 HOMO: -7.06408 LUMO: -1.16737 factor:1 | -1 (0.50523) | 1 | 1 |
| G: -6290.53967 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.24974 HOMO: -6.71849 LUMO: -1.02315 factor:1 | -1 (0.65563) | -1 | -1 |
| G: -6290.53967 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.44525 HOMO: -6.16610 LUMO: -0.50885 factor:1 | -1 (0.46012) | -1 | -1 |
| G: -6290.53967 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.32143 HOMO: -6.48447 LUMO: 0.07619 factor:1 | 1 (-0.41606) | -1 | -1 |
| G: -6290.53967 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12556.03823 HOMO: -7.06135 LUMO: 0.09796 factor:1 | 1 (-1.13286) | 1 | 1 |
| G: -6290.53967 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.97173 HOMO: -6.47359 LUMO: 0.22585 factor:1 | 1 (-1.06636) | -1 | -1 |
| G: -6290.53967 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.33612 HOMO: -6.10896 LUMO: -0.62314 factor:1 | 1 (-0.43076) | -1 | -1 |
| G: -6290.53967 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.81398 HOMO: -6.88176 LUMO: -0.96600 factor:1 | 1 (-0.90862) | -1 | -1 |
| G: -6290.53967 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.16886 HOMO: -6.67495 LUMO: 0.21769 factor:1 | 1 (-0.26349) | -1 | -1 |
| G: -6290.53967 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.36393 HOMO: -6.84911 LUMO: 0.38368 factor:1 | 1 (-0.45857) | -1 | -1 |
| G: -6290.53967 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.28576 HOMO: -6.83550 LUMO: 1.29798 factor:1 | 1 (-0.38039) | -1 | -1 |
| G: -6290.53967 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.25599 HOMO: -6.67495 LUMO: 1.46941 factor:1 | 1 (-0.35062) | -1 | -1 |
| G: -6290.53967 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.29974 HOMO: -6.81917 LUMO: 1.30887 factor:1 | 1 (-0.39437) | -1 | -1 |
| G: -6290.53967 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.93582 HOMO: -6.56611 LUMO: 0.66396 factor:1 | 1 (-0.03045) | -1 | -1 |
| G: -6290.53967 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.07421 HOMO: -6.76203 LUMO: 0.60137 factor:1 | 1 (-0.16885) | -1 | -1 |
| G: -6290.53967 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.04017 HOMO: -6.55794 LUMO: 0.34286 factor:1 | 1 (-0.13481) | -1 | -1 |
| G: -6290.53967 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.86632 HOMO: -6.83550 LUMO: 0.35919 factor:1 | -1 (0.03905) | -1 | -1 |
| G: -6290.53967 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.26083 HOMO: -7.17836 LUMO: 0.63130 factor:1 | 1 (-0.35546) | 1 | 1 |
| G: -6290.53967 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.38555 HOMO: -6.29944 LUMO: -0.69389 factor:1 | -1 (0.51982) | -1 | -1 |
| G: -6290.53967 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.45328 HOMO: -7.06680 LUMO: -0.95784 factor:1 | -1 (0.45209) | 1 | 1 |
| G: -6290.53967 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.25058 HOMO: -6.84638 LUMO: -0.87076 factor:1 | -1 (0.65479) | -1 | -1 |
| G: -6290.53967 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.45698 HOMO: -6.96339 LUMO: -1.05308 factor:1 | -1 (0.44839) | -1 | -1 |
| G: -6290.53967 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.30566 HOMO: -6.75387 LUMO: -1.04220 factor:1 | -1 (0.59971) | -1 | -1 |
| G: -6290.53967 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.44824 HOMO: -6.71849 LUMO: -0.84355 factor:1 | -1 (0.45712) | -1 | -1 |
| G: -6290.53967 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.22242 HOMO: -7.16748 LUMO: 0.51702 factor:1 | -1 (0.68295) | 1 | 1 |
| G: -6290.53967 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.42819 HOMO: -6.92530 LUMO: 0.71566 factor:1 | -1 (0.47718) | -1 | -1 |
| G: -6290.53967 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.32177 HOMO: -7.11034 LUMO: 0.01905 factor:1 | -1 (0.58360) | 1 | -1 |
| G: -6290.53967 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.26503 HOMO: -6.79468 LUMO: 0.77008 factor:1 | -1 (0.64034) | -1 | -1 |
| G: -6290.53967 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.46318 HOMO: -6.52801 LUMO: 0.98233 factor:1 | -1 (0.44219) | -1 | -1 |
| G: -6290.53967 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.29115 HOMO: -6.76475 LUMO: 0.53334 factor:1 | -1 (0.61422) | -1 | -1 |
| G: -6290.53967 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.26315 HOMO: -5.29261 LUMO: 0.57416 factor:1 | -1 (0.64222) | -1 | -1 |
| G: -6290.53967 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.31172 HOMO: -6.57971 LUMO: 0.12789 factor:1 | -1 (0.59364) | -1 | -1 |
| G: -6290.53967 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.23423 HOMO: -6.99333 LUMO: 0.51430 factor:1 | -1 (0.67114) | -1 | -1 |
| G: -6290.53967 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.36865 HOMO: -6.41917 LUMO: 0.19048 factor:1 | -1 (0.53672) | -1 | -1 |
| G: -6290.53967 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.31276 HOMO: -6.16066 LUMO: 1.77146 factor:1 | -1 (0.59261) | -1 | -1 |
| G: -6290.53967 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.51565 HOMO: -6.90353 LUMO: 1.65717 factor:1 | -1 (0.38972) | -1 | -1 |
| G: -6290.53967 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.41026 HOMO: -5.94569 LUMO: 1.29526 factor:1 | -1 (0.49511) | -1 | -1 |
| G: -6290.53967 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.28922 HOMO: -6.60420 LUMO: 1.33880 factor:1 | -1 (0.61615) | -1 | -1 |
| G: -6290.53967 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12553.97528 HOMO: -6.23957 LUMO: 0.09524 factor:1 | -1 (0.93009) | -1 | -1 |
| G: -6290.53967 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.20859 HOMO: -6.80013 LUMO: 1.34696 factor:1 | -1 (0.69677) | -1 | -1 |
| G: -6290.53967 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.40326 HOMO: -7.53483 LUMO: -1.52384 factor:1 | -1 (0.50210) | -1 | -1 |
| G: -6290.53967 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.19643 HOMO: -7.62463 LUMO: -1.65717 factor:1 | -1 (0.70894) | -1 | -1 |
| G: -6290.53967 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.41047 HOMO: -7.62463 LUMO: -1.61364 factor:1 | -1 (0.49489) | -1 | -1 |
| G: -6290.53967 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.32620 HOMO: -8.04096 LUMO: -1.66806 factor:1 | -1 (0.57917) | -1 | -1 |
| G: -6290.53967 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.23409 HOMO: -7.18381 LUMO: -1.17553 factor:1 | -1 (0.67128) | 1 | 1 |
| G: -6290.53967 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.43760 HOMO: -7.69538 LUMO: -1.36601 factor:1 | -1 (0.46776) | 1 | 1 |
| G: -6290.53967 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.50642 HOMO: -7.95117 LUMO: -1.48302 factor:1 | -1 (0.39895) | -1 | -1 |
| G: -6290.53967 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.96665 HOMO: -6.98516 LUMO: 0.35919 factor:1 | 1 (-0.06128) | -1 | -1 |
| G: -6290.53967 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.04978 HOMO: -7.91579 LUMO: -0.32109 factor:1 | 1 (-0.14441) | 1 | 1 |
| G: -6290.53967 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.90112 HOMO: -6.75659 LUMO: -0.03537 factor:1 | -1 (0.00424) | -1 | -1 |
| G: -6290.53967 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.00159 HOMO: -7.78518 LUMO: -2.36467 factor:1 | 1 (-0.09622) | -1 | -1 |
| G: -6290.53967 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.08730 HOMO: -7.96477 LUMO: -2.75651 factor:1 | 1 (-0.18194) | -1 | -1 |
| G: -6290.53967 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.22344 HOMO: -7.60286 LUMO: -2.35106 factor:1 | 1 (-0.31807) | -1 | -1 |
| G: -6290.53967 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.36336 HOMO: -7.38245 LUMO: -1.21635 factor:1 | 1 (-0.45799) | 1 | 1 |
| G: -6290.53967 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.96719 HOMO: -7.91579 LUMO: -1.50479 factor:1 | 1 (-0.06182) | -1 | -1 |
| G: -6290.53967 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.45822 HOMO: -8.07362 LUMO: -0.28028 factor:1 | 1 (-0.55285) | 1 | 1 |
| G: -6290.53967 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12556.38678 HOMO: -7.38245 LUMO: -1.15921 factor:1 | 1 (-1.48142) | 1 | 1 |
| G: -6290.53967 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12556.16795 HOMO: -7.18653 LUMO: -0.94968 factor:1 | 1 (-1.26258) | 1 | 1 |
| G: -6290.53967 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12556.42335 HOMO: -6.88448 LUMO: 0.38096 factor:1 | 1 (-1.51799) | -1 | -1 |
| G: -6290.53967 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.50184 HOMO: -6.97972 LUMO: 0.43266 factor:1 | 1 (-0.59647) | -1 | -1 |
| G: -6290.53967 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12556.01902 HOMO: -6.88992 LUMO: -0.43538 factor:1 | 1 (-1.11365) | -1 | -1 |
| G: -6290.53967 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.41030 HOMO: -7.97021 LUMO: -0.17143 factor:1 | 1 (-0.50493) | 1 | 1 |
| G: -6290.53967 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12556.20528 HOMO: -6.92530 LUMO: 0.77280 factor:1 | 1 (-1.29992) | -1 | -1 |
| G: -6290.53967 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12556.26485 HOMO: -7.89674 LUMO: -0.09796 factor:1 | 1 (-1.35948) | 1 | 1 |
| G: -6290.53967 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.24129 HOMO: -7.02870 LUMO: 0.88709 factor:1 | 1 (-0.33592) | -1 | -1 |
| G: -6290.53967 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12556.05448 HOMO: -6.78380 LUMO: 0.22041 factor:1 | 1 (-1.14911) | -1 | -1 |
| G: -6290.53967 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.45700 HOMO: -7.24911 LUMO: -0.82178 factor:1 | 1 (-0.55163) | 1 | 1 |
| G: -6290.53967 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.27988 HOMO: -6.77019 LUMO: 0.52790 factor:1 | 1 (-0.37451) | -1 | -1 |
| G: -6290.53967 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.18823 HOMO: -8.56070 LUMO: -1.83405 factor:1 | 1 (-0.28286) | -1 | -1 |
| G: -6290.53967 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.34099 HOMO: -7.74164 LUMO: -2.36195 factor:1 | 1 (-0.43563) | -1 | -1 |
| G: -6290.53967 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.40932 HOMO: -7.39878 LUMO: -2.41637 factor:1 | 1 (-0.50395) | -1 | -1 |
| G: -6290.53967 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.26045 HOMO: -7.61647 LUMO: -2.34018 factor:1 | 1 (-0.35508) | -1 | -1 |
| G: -6290.53967 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.96940 HOMO: -6.93346 LUMO: -0.57688 factor:1 | 1 (-0.06403) | -1 | -1 |
| G: -6290.53967 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.46758 HOMO: -6.85183 LUMO: -1.00410 factor:1 | 1 (-0.56221) | -1 | -1 |
| G: -6290.53967 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.38114 HOMO: -7.18925 LUMO: -1.12655 factor:1 | -1 (0.52423) | 1 | 1 |
| G: -6290.53967 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.39728 HOMO: -6.85183 LUMO: -1.60275 factor:1 | -1 (0.50809) | -1 | -1 |
| G: -6290.53967 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.35328 HOMO: -7.51578 LUMO: 0.12517 factor:1 | -1 (0.55209) | 1 | 1 |
| G: -6290.53967 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12553.98236 HOMO: -7.36068 LUMO: 0.05714 factor:1 | -1 (0.92301) | 1 | 1 |
| G: -6290.53967 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.16582 HOMO: -7.49674 LUMO: 0.18776 factor:1 | -1 (0.73955) | 1 | 1 |
| G: -6290.53967 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.25055 HOMO: -7.09401 LUMO: -1.24900 factor:1 | -1 (0.65481) | 1 | 1 |
| G: -6290.53967 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12553.91675 HOMO: -7.22462 LUMO: -1.61364 factor:1 | -1 (0.98862) | -1 | -1 |
| G: -6290.53967 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.11776 HOMO: -7.74436 LUMO: -0.18776 factor:1 | -1 (0.78761) | 1 | 1 |
| G: -6290.53967 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.27458 HOMO: -7.35252 LUMO: 0.75376 factor:1 | -1 (0.63079) | 1 | 1 |
| G: -6290.53967 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.17681 HOMO: -7.75252 LUMO: 0.00816 factor:1 | -1 (0.72856) | 1 | 1 |
| G: -6290.53967 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.62326 HOMO: -7.06680 LUMO: 0.24490 factor:1 | 1 (-0.71789) | 1 | 1 |
| G: -6290.53967 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.35580 HOMO: -7.49129 LUMO: 0.14150 factor:1 | 1 (-0.45043) | 1 | 1 |
| G: -6290.53967 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12556.39514 HOMO: -6.90625 LUMO: -1.11295 factor:1 | 1 (-1.48977) | -1 | -1 |
| G: -6290.53967 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12556.30681 HOMO: -6.78380 LUMO: -0.93063 factor:1 | 1 (-1.40144) | -1 | -1 |
| G: -6290.53967 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12556.17853 HOMO: -7.79878 LUMO: 0.30477 factor:1 | 1 (-1.27317) | 1 | 1 |
| G: -6290.53967 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.19373 HOMO: -7.87498 LUMO: 0.61770 factor:1 | 1 (-0.28836) | 1 | 1 |
| G: -6290.53967 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12553.87792 HOMO: -7.23823 LUMO: 0.30205 factor:1 | -1 (1.02745) | 1 | 1 |
| G: -6290.53967 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.09156 HOMO: -7.67633 LUMO: 0.13061 factor:1 | -1 (0.81381) | 1 | 1 |
| G: -6290.53967 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.24691 HOMO: -7.79606 LUMO: 0.34558 factor:1 | -1 (0.65846) | 1 | 1 |
| G: -6290.53967 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.83445 HOMO: -6.66135 LUMO: -2.60141 factor:1 | 1 (-0.92908) | -1 | -1 |
| G: -6290.53967 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.80266 HOMO: -7.03142 LUMO: 0.50885 factor:1 | 1 (-0.89730) | -1 | -1 |
| G: -6290.53967 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.00401 HOMO: -7.05591 LUMO: -0.06531 factor:1 | 1 (-0.09864) | -1 | -1 |
| G: -6290.53967 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.69183 HOMO: -7.45592 LUMO: -1.39594 factor:1 | 1 (-0.78646) | 1 | 1 |
| G: -6290.53967 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.87652 HOMO: -7.22462 LUMO: -1.10478 factor:1 | -1 (0.02884) | 1 | 1 |
| G: -6290.53967 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.90262 HOMO: -8.14709 LUMO: -0.55783 factor:1 | -1 (0.00275) | 1 | 1 |
| G: -6290.53967 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.88136 HOMO: -7.22190 LUMO: -1.14560 factor:1 | 1 (-0.97599) | 1 | 1 |
| G: -6290.53967 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.09870 HOMO: -7.28721 LUMO: -1.14016 factor:1 | 1 (-0.19334) | 1 | 1 |
| G: -6290.53967 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.11990 HOMO: -6.97156 LUMO: 0.51702 factor:1 | 1 (-0.21453) | -1 | -1 |
| G: -6290.53967 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.23016 HOMO: -7.37156 LUMO: 0.29388 factor:1 | 1 (-0.32480) | 1 | -1 |
| G: -6290.45426 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.24925 HOMO: -7.66273 LUMO: -1.59731 factor:1 | -1 (0.57070) | -1 | -1 |
| G: -6290.45426 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.74863 HOMO: -7.50490 LUMO: -1.49935 factor:1 | -1 (0.07132) | -1 | -1 |
| G: -6290.45426 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12556.64135 HOMO: -7.61102 LUMO: -1.45581 factor:1 | 1 (-1.82139) | 1 | 1 |
| G: -6290.45426 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12556.08155 HOMO: -7.58653 LUMO: -1.61091 factor:1 | 1 (-1.26160) | -1 | -1 |
| G: -6290.45426 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.70810 HOMO: -7.36068 LUMO: -1.14560 factor:1 | 1 (-0.88815) | 1 | 1 |
| G: -6290.45426 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.66202 HOMO: -6.96339 LUMO: 0.26939 factor:1 | -1 (0.15793) | -1 | -1 |
| G: -6290.45426 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.40056 HOMO: -6.53617 LUMO: 0.22313 factor:1 | 1 (-0.58061) | -1 | -1 |
| G: -6290.45426 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.48611 HOMO: -7.33619 LUMO: -1.02587 factor:1 | 1 (-0.66616) | 1 | 1 |
| G: -6290.45426 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12556.10906 HOMO: -6.87904 LUMO: 0.33742 factor:1 | 1 (-1.28911) | -1 | -1 |
| G: -6290.45426 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.41662 HOMO: -6.88448 LUMO: 0.58777 factor:1 | 1 (-0.59666) | -1 | -1 |
| G: -6290.45426 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.97246 HOMO: -6.55522 LUMO: -1.51295 factor:1 | 1 (-1.15251) | -1 | -1 |
| G: -6290.45426 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12556.00275 HOMO: -7.43415 LUMO: 0.10612 factor:1 | 1 (-1.18280) | 1 | 1 |
| G: -6290.45426 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.69451 HOMO: -7.54300 LUMO: -0.02449 factor:1 | -1 (0.12544) | 1 | 1 |
| G: -6290.45426 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12556.08310 HOMO: -7.42054 LUMO: 0.28028 factor:1 | 1 (-1.26315) | 1 | 1 |
| G: -6290.45426 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.54884 HOMO: -6.98244 LUMO: -0.95784 factor:1 | 1 (-0.72888) | -1 | -1 |
| G: -6290.45426 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.59148 HOMO: -6.96884 LUMO: -1.12383 factor:1 | 1 (-0.77152) | -1 | -1 |
| G: -6290.45426 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.59877 HOMO: -6.80829 LUMO: -0.98233 factor:1 | 1 (-0.77882) | -1 | -1 |
| G: -6290.45426 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.65365 HOMO: -7.60830 LUMO: 0.58504 factor:1 | 1 (-0.83370) | 1 | 1 |
| G: -6290.45426 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.71919 HOMO: -7.52123 LUMO: 0.08163 factor:1 | -1 (0.10076) | 1 | 1 |
| G: -6290.45426 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.70757 HOMO: -7.59742 LUMO: 0.00272 factor:1 | -1 (0.11238) | 1 | 1 |
| G: -6290.45426 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.61769 HOMO: -6.99333 LUMO: -1.33880 factor:1 | -1 (0.20226) | -1 | -1 |
| G: -6290.45426 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.72281 HOMO: -6.63958 LUMO: -1.39322 factor:1 | -1 (0.09714) | -1 | -1 |
| G: -6290.45426 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.70787 HOMO: -7.86137 LUMO: 0.01633 factor:1 | -1 (0.11208) | 1 | 1 |
| G: -6290.45426 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.46174 HOMO: -7.29537 LUMO: 0.14694 factor:1 | -1 (0.35821) | 1 | 1 |
| G: -6290.45426 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12556.68480 HOMO: -6.95523 LUMO: 0.48708 factor:1 | 1 (-1.86485) | -1 | -1 |
| G: -6290.45426 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.88345 HOMO: -7.10217 LUMO: -1.10478 factor:1 | 1 (-1.06350) | 1 | 1 |
| G: -6290.45426 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.54762 HOMO: -6.88176 LUMO: -0.96328 factor:1 | -1 (0.27233) | -1 | -1 |
| G: -6290.45426 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.96054 HOMO: -7.89130 LUMO: -0.13334 factor:1 | 1 (-1.14059) | 1 | 1 |
| G: -6290.45426 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12556.01973 HOMO: -7.75252 LUMO: 0.25579 factor:1 | 1 (-1.19978) | 1 | 1 |
| G: -6290.45426 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.38168 HOMO: -6.87632 LUMO: -0.93063 factor:1 | 1 (-0.56172) | -1 | -1 |
| G: -6290.45426 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.54633 HOMO: -6.78108 LUMO: -0.86804 factor:1 | 1 (-0.72638) | -1 | -1 |
| G: -6290.45426 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.49572 HOMO: -5.98106 LUMO: 0.10340 factor:1 | 1 (-0.67577) | -1 | -1 |
| G: -6290.45426 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.54122 HOMO: -6.40284 LUMO: -0.87349 factor:1 | -1 (0.27873) | -1 | -1 |
| G: -6290.45426 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.57461 HOMO: -6.77019 LUMO: -1.20819 factor:1 | -1 (0.24534) | -1 | -1 |
| G: -6290.45426 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.67320 HOMO: -6.90081 LUMO: -1.00682 factor:1 | -1 (0.14675) | -1 | -1 |
| G: -6290.45426 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.86651 HOMO: -6.59060 LUMO: -0.26667 factor:1 | 1 (-0.04656) | -1 | -1 |
| G: -6290.45426 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.87571 HOMO: -6.50896 LUMO: -0.48708 factor:1 | 1 (-0.05576) | -1 | -1 |
| G: -6290.45426 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.81622 HOMO: -6.20420 LUMO: -0.73471 factor:1 | -1 (0.00373) | -1 | -1 |
| G: -6290.45426 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.97568 HOMO: -6.17154 LUMO: -0.68573 factor:1 | 1 (-0.15573) | -1 | -1 |
| G: -6290.45426 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.78226 HOMO: -6.21236 LUMO: 0.09796 factor:1 | -1 (0.03769) | -1 | -1 |
| G: -6290.45426 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.38744 HOMO: -6.38379 LUMO: 0.58232 factor:1 | 1 (-0.56749) | -1 | -1 |
| G: -6290.45426 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.52130 HOMO: -7.42871 LUMO: 0.40273 factor:1 | 1 (-0.70135) | 1 | 1 |
| G: -6290.45426 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.29925 HOMO: -6.54978 LUMO: 0.26395 factor:1 | 1 (-0.47930) | -1 | -1 |
| G: -6290.45426 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.67130 HOMO: -7.14027 LUMO: 0.14150 factor:1 | -1 (0.14866) | 1 | 1 |
| G: -6290.45426 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.65012 HOMO: -7.25456 LUMO: -0.15783 factor:1 | -1 (0.16983) | 1 | 1 |
| G: -6290.45426 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.82164 HOMO: -6.90897 LUMO: 0.63403 factor:1 | 1 (-0.00169) | -1 | -1 |
| G: -6290.45426 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.69924 HOMO: -6.49264 LUMO: 0.71022 factor:1 | -1 (0.12071) | -1 | -1 |
| G: -6290.45426 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.75658 HOMO: -6.56067 LUMO: -1.03947 factor:1 | -1 (0.06338) | -1 | -1 |
| G: -6290.45426 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.69048 HOMO: -6.79196 LUMO: -1.12655 factor:1 | -1 (0.12947) | -1 | -1 |
| G: -6290.45426 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.39765 HOMO: -6.95251 LUMO: -1.09118 factor:1 | 1 (-0.57770) | -1 | -1 |
| G: -6290.45426 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.60682 HOMO: -7.47225 LUMO: -0.22041 factor:1 | 1 (-0.78687) | 1 | 1 |
| G: -6290.45426 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.54734 HOMO: -7.13483 LUMO: -0.98505 factor:1 | 1 (-0.72739) | 1 | 1 |
| G: -6290.45426 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.77078 HOMO: -6.99061 LUMO: -1.05852 factor:1 | -1 (0.04917) | -1 | -1 |
| G: -6290.45426 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.25792 HOMO: -6.52257 LUMO: -1.11022 factor:1 | 1 (-0.43797) | -1 | -1 |
| G: -6290.45426 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.38347 HOMO: -6.75114 LUMO: -1.09934 factor:1 | 1 (-0.56352) | -1 | -1 |
| G: -6290.45426 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.34524 HOMO: -6.82189 LUMO: -0.89253 factor:1 | 1 (-0.52529) | -1 | -1 |
| G: -6290.45426 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.41803 HOMO: -6.83278 LUMO: -0.97961 factor:1 | 1 (-0.59808) | -1 | -1 |
| G: -6290.45426 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.18524 HOMO: -6.65318 LUMO: -0.84355 factor:1 | 1 (-0.36529) | -1 | -1 |
| G: -6290.45426 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.19827 HOMO: -6.75931 LUMO: -0.88437 factor:1 | 1 (-0.37832) | -1 | -1 |
| G: -6290.45426 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.47436 HOMO: -6.19059 LUMO: -0.45715 factor:1 | 1 (-0.65441) | -1 | -1 |
| G: -6290.45426 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12556.70061 HOMO: -7.09673 LUMO: -2.01908 factor:1 | 1 (-1.88066) | -1 | -1 |
| G: -6290.45426 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.93363 HOMO: -7.88042 LUMO: 0.38640 factor:1 | 1 (-1.11368) | 1 | 1 |
| G: -6290.45426 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.71648 HOMO: -7.83144 LUMO: 0.14422 factor:1 | 1 (-0.89653) | 1 | 1 |
| G: -6290.45426 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12556.07206 HOMO: -7.46408 LUMO: 0.44627 factor:1 | 1 (-1.25210) | 1 | 1 |
| G: -6290.45426 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.70281 HOMO: -7.12394 LUMO: -2.04902 factor:1 | -1 (0.11715) | -1 | -1 |
| G: -6290.45426 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12556.21807 HOMO: -6.78380 LUMO: -1.11295 factor:1 | 1 (-1.39812) | -1 | -1 |
| G: -6290.45426 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.67232 HOMO: -7.12938 LUMO: -0.23674 factor:1 | 1 (-0.85237) | 1 | 1 |
| G: -6290.45426 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.76468 HOMO: -6.14705 LUMO: -0.20409 factor:1 | -1 (0.05527) | -1 | -1 |
| G: -6290.45426 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.61064 HOMO: -6.50080 LUMO: -0.28300 factor:1 | -1 (0.20931) | -1 | -1 |
| G: -6290.45426 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.39020 HOMO: -6.50352 LUMO: -0.62042 factor:1 | -1 (0.42975) | -1 | -1 |
| G: -6290.45426 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.53635 HOMO: -6.46543 LUMO: -0.53879 factor:1 | -1 (0.28360) | -1 | -1 |
| G: -6290.45426 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.68678 HOMO: -7.32803 LUMO: -0.52790 factor:1 | -1 (0.13317) | 1 | 1 |
| G: -6290.45426 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.26336 HOMO: -5.94025 LUMO: -0.17687 factor:1 | 1 (-0.44341) | -1 | -1 |
| G: -6290.45426 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.31811 HOMO: -5.62187 LUMO: 0.05714 factor:1 | 1 (-0.49816) | -1 | -1 |
| G: -6290.45426 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.49142 HOMO: -7.03414 LUMO: -1.04492 factor:1 | 1 (-0.67147) | -1 | -1 |
| G: -6290.45426 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.65447 HOMO: -6.75387 LUMO: -2.02181 factor:1 | 1 (-0.83452) | -1 | -1 |
| G: -6290.45426 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.40562 HOMO: -6.55250 LUMO: -0.75648 factor:1 | 1 (-0.58567) | -1 | -1 |
| G: -6290.45426 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.35355 HOMO: -6.81101 LUMO: -1.02043 factor:1 | -1 (0.46640) | -1 | -1 |
| G: -6290.45426 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.34291 HOMO: -6.69672 LUMO: -2.81910 factor:1 | -1 (0.47704) | -1 | -1 |
| G: -6290.45426 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12556.55971 HOMO: -6.69128 LUMO: -2.58236 factor:1 | 1 (-1.73976) | -1 | -1 |
| G: -6290.45426 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.65673 HOMO: -6.73482 LUMO: -2.06807 factor:1 | 1 (-0.83678) | -1 | -1 |
| G: -6290.45426 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.31529 HOMO: -7.66545 LUMO: 0.17143 factor:1 | -1 (0.50466) | 1 | 1 |
| G: -6290.45426 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.92762 HOMO: -6.87904 LUMO: -1.25172 factor:1 | 1 (-1.10767) | -1 | -1 |
| G: -6290.45426 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12556.04014 HOMO: -6.84366 LUMO: -0.19320 factor:1 | 1 (-1.22019) | -1 | -1 |
| G: -6290.45426 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.26508 HOMO: -6.97972 LUMO: -0.97961 factor:1 | 1 (-0.44512) | -1 | -1 |
| G: -6290.45426 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.28399 HOMO: -6.72121 LUMO: -0.70477 factor:1 | 1 (-0.46404) | -1 | -1 |
| G: -6290.45426 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.66449 HOMO: -7.18925 LUMO: 0.40001 factor:1 | -1 (0.15546) | 1 | 1 |
| G: -6290.45426 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.76854 HOMO: -6.72121 LUMO: 0.19592 factor:1 | 1 (-0.94859) | -1 | -1 |
| G: -6290.45426 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.67120 HOMO: -6.85999 LUMO: -0.39457 factor:1 | 1 (-0.85125) | -1 | -1 |
| G: -6290.45426 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12556.20950 HOMO: -6.90625 LUMO: 0.05987 factor:1 | 1 (-1.38955) | -1 | -1 |
| G: -6290.45426 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.89138 HOMO: -7.00421 LUMO: 0.37552 factor:1 | 1 (-0.07143) | -1 | -1 |
| G: -6290.45426 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.41596 HOMO: -6.56883 LUMO: -0.97689 factor:1 | 1 (-0.59601) | -1 | -1 |
| G: -6290.45426 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.24475 HOMO: -6.66679 LUMO: 0.56055 factor:1 | 1 (-0.42480) | -1 | -1 |
| G: -6290.45426 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.00872 HOMO: -6.75931 LUMO: 0.32926 factor:1 | 1 (-0.18877) | -1 | -1 |
| G: -6290.45426 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.95936 HOMO: -6.53617 LUMO: -1.06397 factor:1 | 1 (-0.13940) | -1 | -1 |
| G: -6290.45426 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.92877 HOMO: -6.78108 LUMO: 0.42722 factor:1 | 1 (-0.10882) | -1 | -1 |
| G: -6290.45426 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.12213 HOMO: -7.05319 LUMO: 0.61498 factor:1 | 1 (-0.30218) | -1 | -1 |
| G: -6290.45426 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.97280 HOMO: -6.78380 LUMO: 1.49391 factor:1 | 1 (-0.15285) | -1 | -1 |
| G: -6290.45426 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.79601 HOMO: -7.21102 LUMO: 0.27211 factor:1 | -1 (0.02395) | 1 | 1 |
| G: -6290.45426 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.84499 HOMO: -6.67223 LUMO: 0.81362 factor:1 | 1 (-0.02503) | -1 | -1 |
| G: -6290.45426 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.54622 HOMO: -6.69944 LUMO: 1.40683 factor:1 | 1 (-0.72627) | -1 | -1 |
| G: -6290.45426 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.50007 HOMO: -7.02598 LUMO: 1.46941 factor:1 | 1 (-0.68012) | -1 | -1 |
| G: -6290.45426 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.36304 HOMO: -5.85045 LUMO: -0.76736 factor:1 | 1 (-0.54308) | -1 | -1 |
| G: -6290.45426 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.65281 HOMO: -6.53890 LUMO: -0.50885 factor:1 | 1 (-0.83286) | -1 | -1 |
| G: -6290.45426 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.49479 HOMO: -6.42733 LUMO: -0.63947 factor:1 | 1 (-0.67484) | -1 | -1 |
| G: -6290.45426 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.53417 HOMO: -6.82189 LUMO: -0.85444 factor:1 | 1 (-0.71422) | -1 | -1 |
| G: -6290.45426 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.63851 HOMO: -6.97428 LUMO: -1.22179 factor:1 | -1 (0.18145) | -1 | -1 |
| G: -6290.45426 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.46551 HOMO: -6.93346 LUMO: -1.09934 factor:1 | 1 (-0.64556) | -1 | -1 |
| G: -6290.45426 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.61232 HOMO: -7.17292 LUMO: -1.11839 factor:1 | 1 (-0.79237) | 1 | 1 |
| G: -6290.45426 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.45950 HOMO: -7.00965 LUMO: -1.23268 factor:1 | 1 (-0.63955) | -1 | -1 |
| G: -6290.45426 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.42383 HOMO: -6.73210 LUMO: -1.12383 factor:1 | 1 (-0.60388) | -1 | -1 |
| G: -6290.45426 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.69110 HOMO: -7.61375 LUMO: -0.11973 factor:1 | 1 (-0.87115) | 1 | 1 |
| G: -6290.45426 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.57724 HOMO: -7.42327 LUMO: 0.41906 factor:1 | 1 (-0.75729) | 1 | 1 |
| G: -6290.45426 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.68906 HOMO: -6.94162 LUMO: -1.01771 factor:1 | 1 (-0.86910) | -1 | -1 |
| G: -6290.45426 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.50249 HOMO: -6.82189 LUMO: -0.92791 factor:1 | 1 (-0.68254) | -1 | -1 |
| G: -6290.45426 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.61806 HOMO: -6.92258 LUMO: -1.73881 factor:1 | 1 (-0.79811) | -1 | -1 |
| G: -6290.45426 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.42007 HOMO: -6.50896 LUMO: -1.60819 factor:1 | 1 (-0.60012) | -1 | -1 |
| G: -6290.45426 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.34780 HOMO: -6.38379 LUMO: -2.18780 factor:1 | 1 (-0.52785) | -1 | -1 |
| G: -6290.45426 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.72836 HOMO: -6.48992 LUMO: -0.97417 factor:1 | -1 (0.09159) | -1 | -1 |
| G: -6290.45426 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.44113 HOMO: -6.01644 LUMO: -0.04354 factor:1 | 1 (-0.62118) | -1 | -1 |
| G: -6290.45426 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.36889 HOMO: -6.70761 LUMO: -0.14422 factor:1 | 1 (-0.54894) | -1 | -1 |
| G: -6290.45426 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.38940 HOMO: -6.70216 LUMO: 0.14422 factor:1 | 1 (-0.56945) | -1 | -1 |
| G: -6290.45426 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.48356 HOMO: -7.07224 LUMO: -0.10885 factor:1 | 1 (-0.66360) | 1 | 1 |
| G: -6290.45426 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.59907 HOMO: -7.52667 LUMO: -0.74287 factor:1 | 1 (-0.77912) | 1 | 1 |
| G: -6290.45426 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.71172 HOMO: -6.48447 LUMO: -0.96056 factor:1 | 1 (-0.89177) | -1 | -1 |
| G: -6290.45426 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.87701 HOMO: -6.22597 LUMO: -0.41361 factor:1 | 1 (-0.05706) | -1 | -1 |
| G: -6290.45426 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.32080 HOMO: -6.12256 LUMO: -1.05852 factor:1 | 1 (-0.50085) | -1 | -1 |
| G: -6290.45426 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.98714 HOMO: -6.97428 LUMO: -0.60681 factor:1 | 1 (-0.16719) | -1 | -1 |
| G: -6290.45426 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.27427 HOMO: -6.78380 LUMO: -0.88981 factor:1 | 1 (-0.45432) | -1 | -1 |
| G: -6290.45426 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.02586 HOMO: -6.85999 LUMO: 0.07891 factor:1 | 1 (-0.20591) | -1 | -1 |
| G: -6290.45426 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.39237 HOMO: -7.08312 LUMO: -0.60137 factor:1 | 1 (-0.57242) | 1 | 1 |
| G: -6290.45426 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.46897 HOMO: -6.57699 LUMO: -0.68028 factor:1 | 1 (-0.64902) | -1 | -1 |
| G: -6290.45426 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.46252 HOMO: -6.09807 LUMO: -0.31837 factor:1 | 1 (-0.64257) | -1 | -1 |
| G: -6290.45426 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.44023 HOMO: -6.10624 LUMO: 0.14966 factor:1 | 1 (-0.62028) | -1 | -1 |
| G: -6290.45426 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.04311 HOMO: -6.77019 LUMO: -0.95784 factor:1 | 1 (-0.22316) | -1 | -1 |
| G: -6290.45426 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.00779 HOMO: -5.93208 LUMO: -0.44627 factor:1 | 1 (-0.18784) | -1 | -1 |
| G: -6290.45426 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.26616 HOMO: -6.12256 LUMO: -0.27756 factor:1 | 1 (-0.44621) | -1 | -1 |
| G: -6290.45426 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.14711 HOMO: -5.98106 LUMO: -0.37824 factor:1 | 1 (-0.32716) | -1 | -1 |
| G: -6290.45426 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.10635 HOMO: -7.06408 LUMO: -1.12927 factor:1 | 1 (-0.28640) | 1 | 1 |
| G: -6290.45426 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.73323 HOMO: -6.70761 LUMO: -0.98505 factor:1 | -1 (0.08672) | -1 | -1 |
| G: -6290.45426 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.92801 HOMO: -7.00965 LUMO: -0.42722 factor:1 | 1 (-0.10806) | -1 | -1 |
| G: -6290.45426 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.91440 HOMO: -5.96201 LUMO: -0.59049 factor:1 | 1 (-0.09445) | -1 | -1 |
| G: -6290.45426 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.85573 HOMO: -6.34570 LUMO: -1.68438 factor:1 | 1 (-0.03578) | -1 | -1 |
| G: -6290.45426 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.48422 HOMO: -6.97156 LUMO: -1.85854 factor:1 | -1 (0.33573) | -1 | -1 |
| G: -6290.45426 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.99331 HOMO: -5.91848 LUMO: -2.51433 factor:1 | 1 (-0.17336) | -1 | -1 |
| G: -6290.45426 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.62117 HOMO: -6.39195 LUMO: -1.66262 factor:1 | -1 (0.19878) | -1 | -1 |
| G: -6290.45426 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.35904 HOMO: -6.50352 LUMO: 0.19592 factor:1 | 1 (-0.53908) | -1 | -1 |
| G: -6290.45426 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.89507 HOMO: -6.45998 LUMO: 0.34831 factor:1 | 1 (-1.07512) | -1 | -1 |
| G: -6290.45426 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.85657 HOMO: -7.05319 LUMO: 0.23402 factor:1 | 1 (-1.03662) | -1 | -1 |
| G: -6290.45426 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12556.42352 HOMO: -6.61237 LUMO: 0.18232 factor:1 | 1 (-1.60357) | -1 | -1 |
| G: -6290.45426 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12556.25546 HOMO: -6.57427 LUMO: 0.40545 factor:1 | 1 (-1.43551) | -1 | -1 |
| G: -6290.45426 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.93594 HOMO: -7.26544 LUMO: 0.41089 factor:1 | 1 (-1.11599) | 1 | 1 |
| G: -6290.45426 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.54247 HOMO: -6.26406 LUMO: -0.85444 factor:1 | 1 (-0.72252) | -1 | -1 |
| G: -6290.45426 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.85921 HOMO: -6.25318 LUMO: -0.79457 factor:1 | 1 (-1.03926) | -1 | -1 |
| G: -6290.45426 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.81126 HOMO: -6.68040 LUMO: 0.41089 factor:1 | 1 (-0.99131) | -1 | -1 |
| G: -6290.45426 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12556.06357 HOMO: -6.37835 LUMO: 0.37280 factor:1 | 1 (-1.24361) | -1 | -1 |
| G: -6290.45426 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12556.39748 HOMO: -6.56067 LUMO: 0.62858 factor:1 | 1 (-1.57753) | -1 | -1 |
| G: -6290.45426 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12556.39677 HOMO: -6.74026 LUMO: -0.04082 factor:1 | 1 (-1.57682) | -1 | -1 |
| G: -6290.45426 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12556.55440 HOMO: -6.53617 LUMO: 0.35103 factor:1 | 1 (-1.73445) | -1 | -1 |
| G: -6290.45426 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.91496 HOMO: -6.51985 LUMO: 0.25851 factor:1 | 1 (-1.09501) | -1 | -1 |
| G: -6290.45426 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12556.60692 HOMO: -6.58788 LUMO: -1.98371 factor:1 | 1 (-1.78697) | -1 | -1 |
| G: -6290.45426 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12556.45731 HOMO: -6.51441 LUMO: 0.29116 factor:1 | 1 (-1.63736) | -1 | -1 |
| G: -6290.45426 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.65442 HOMO: -6.81101 LUMO: 0.35647 factor:1 | 1 (-0.83446) | -1 | -1 |
| G: -6290.45426 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.88794 HOMO: -6.42733 LUMO: 0.10340 factor:1 | 1 (-1.06799) | -1 | -1 |
| G: -6290.45426 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12556.57098 HOMO: -6.70761 LUMO: 0.28028 factor:1 | 1 (-1.75103) | -1 | -1 |
| G: -6290.45426 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12556.44131 HOMO: -6.67495 LUMO: 0.01633 factor:1 | 1 (-1.62136) | -1 | -1 |
| G: -6290.45426 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12556.10923 HOMO: -6.75387 LUMO: 0.15510 factor:1 | 1 (-1.28928) | -1 | -1 |
| G: -6290.45426 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.84634 HOMO: -6.56067 LUMO: 0.35919 factor:1 | 1 (-1.02639) | -1 | -1 |
| G: -6290.45426 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.55694 HOMO: -7.16748 LUMO: 0.21497 factor:1 | 1 (-0.73699) | 1 | 1 |
| G: -6290.45426 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.41551 HOMO: -6.71849 LUMO: 0.26667 factor:1 | -1 (0.40444) | -1 | -1 |
| G: -6290.45426 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.28005 HOMO: -6.69128 LUMO: 0.55783 factor:1 | -1 (0.53990) | -1 | -1 |
| G: -6290.45426 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.44350 HOMO: -6.71305 LUMO: 0.45987 factor:1 | 1 (-0.62355) | -1 | -1 |
| G: -6290.45426 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.49281 HOMO: -5.90487 LUMO: -0.70750 factor:1 | 1 (-0.67286) | -1 | -1 |
| G: -6290.45426 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.68609 HOMO: -6.84638 LUMO: -0.72110 factor:1 | 1 (-0.86614) | -1 | -1 |
| G: -6290.45426 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.37958 HOMO: -6.66135 LUMO: -1.13471 factor:1 | 1 (-0.55963) | -1 | -1 |
| G: -6290.45426 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.79856 HOMO: -6.74026 LUMO: -0.64763 factor:1 | -1 (0.02139) | -1 | -1 |
| G: -6290.45426 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.65685 HOMO: -6.69672 LUMO: -1.05036 factor:1 | -1 (0.16311) | -1 | -1 |
| G: -6290.45426 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.57687 HOMO: -6.78924 LUMO: -1.03675 factor:1 | -1 (0.24308) | -1 | -1 |
| G: -6290.45426 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.75309 HOMO: -6.81373 LUMO: -0.85988 factor:1 | -1 (0.06686) | -1 | -1 |
| G: -6290.45426 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.74934 HOMO: -7.26544 LUMO: 0.91158 factor:1 | -1 (0.07061) | 1 | 1 |
| G: -6290.45426 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.45328 HOMO: -6.64230 LUMO: -1.92929 factor:1 | -1 (0.36667) | -1 | -1 |
| G: -6290.45426 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12556.04680 HOMO: -7.20830 LUMO: 0.11429 factor:1 | 1 (-1.22685) | 1 | 1 |
| G: -6290.45426 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12556.48874 HOMO: -7.17020 LUMO: 0.04898 factor:1 | 1 (-1.66879) | 1 | 1 |
| G: -6290.45426 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.55527 HOMO: -7.16476 LUMO: 0.04898 factor:1 | -1 (0.26469) | 1 | 1 |
| G: -6290.45426 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.89015 HOMO: -6.59332 LUMO: -0.49253 factor:1 | 1 (-1.07020) | -1 | -1 |
| G: -6290.45426 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.23318 HOMO: -7.46953 LUMO: 0.84083 factor:1 | 1 (-0.41323) | 1 | 1 |
| G: -6290.45426 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.55499 HOMO: -7.39878 LUMO: 0.88709 factor:1 | 1 (-0.73503) | 1 | 1 |
| G: -6290.45426 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12556.12569 HOMO: -6.84094 LUMO: -0.61498 factor:1 | 1 (-1.30574) | -1 | -1 |
| G: -6290.45426 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.77570 HOMO: -6.03549 LUMO: -0.27211 factor:1 | 1 (-0.95575) | -1 | -1 |
| G: -6290.45426 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.51722 HOMO: -7.31170 LUMO: -0.64763 factor:1 | 1 (-0.69726) | 1 | 1 |
| G: -6290.45426 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.43194 HOMO: -6.88992 LUMO: -0.84627 factor:1 | 1 (-0.61198) | -1 | -1 |
| G: -6290.45426 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.58217 HOMO: -7.12666 LUMO: -0.09252 factor:1 | 1 (-0.76222) | 1 | 1 |
| G: -6290.45426 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.21248 HOMO: -6.70489 LUMO: -0.63675 factor:1 | 1 (-0.39252) | -1 | -1 |
| G: -6290.45426 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.55833 HOMO: -6.98788 LUMO: 0.86804 factor:1 | 1 (-0.73838) | -1 | -1 |
| G: -6290.45426 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.85545 HOMO: -6.80285 LUMO: -0.60954 factor:1 | 1 (-1.03550) | -1 | -1 |
| G: -6290.45426 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.42883 HOMO: -7.02054 LUMO: -0.74287 factor:1 | 1 (-0.60888) | -1 | -1 |
| G: -6290.45426 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.27749 HOMO: -7.03686 LUMO: -0.81090 factor:1 | -1 (0.54246) | -1 | -1 |
| G: -6290.45426 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.46408 HOMO: -6.70489 LUMO: -1.00954 factor:1 | -1 (0.35587) | -1 | -1 |
| G: -6290.45426 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12553.99694 HOMO: -7.69810 LUMO: 0.00544 factor:1 | -1 (0.82301) | 1 | 1 |
| G: -6290.45426 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.56631 HOMO: -6.83550 LUMO: -0.11157 factor:1 | -1 (0.25364) | -1 | -1 |
| G: -6290.45426 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.33210 HOMO: -6.76203 LUMO: -2.13609 factor:1 | 1 (-0.51215) | -1 | -1 |
| G: -6290.45426 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.94101 HOMO: -6.72121 LUMO: -2.62862 factor:1 | 1 (-1.12105) | -1 | -1 |
| G: -6290.45426 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.48211 HOMO: -6.48719 LUMO: -2.73474 factor:1 | 1 (-0.66216) | -1 | -1 |
| G: -6290.45426 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.18861 HOMO: -6.83006 LUMO: -0.00544 factor:1 | 1 (-0.36866) | -1 | -1 |
| G: -6290.45426 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.86854 HOMO: -6.84094 LUMO: -1.11022 factor:1 | 1 (-1.04859) | -1 | -1 |
| G: -6290.45426 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.79665 HOMO: -6.66951 LUMO: -1.23812 factor:1 | 1 (-0.97670) | -1 | -1 |
| G: -6290.45426 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.95600 HOMO: -6.78380 LUMO: -1.27894 factor:1 | 1 (-1.13605) | -1 | -1 |
| G: -6290.45426 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.59431 HOMO: -6.50352 LUMO: -0.56055 factor:1 | 1 (-0.77435) | -1 | -1 |
| G: -6290.45426 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.42780 HOMO: -7.77974 LUMO: -0.26395 factor:1 | 1 (-0.60785) | 1 | 1 |
| G: -6290.45426 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.37030 HOMO: -7.01510 LUMO: -1.64085 factor:1 | 1 (-0.55035) | -1 | -1 |
| G: -6290.45426 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.71711 HOMO: -6.59876 LUMO: -0.91158 factor:1 | 1 (-0.89716) | -1 | -1 |
| G: -6290.45426 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.42543 HOMO: -4.67219 LUMO: -0.67756 factor:1 | 1 (-0.60548) | -1 | -1 |
| G: -6290.45426 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.78242 HOMO: -6.70489 LUMO: -0.65579 factor:1 | 1 (-0.96247) | -1 | -1 |
| G: -6290.45426 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.82971 HOMO: -6.62325 LUMO: -0.60409 factor:1 | 1 (-1.00976) | -1 | -1 |
| G: -6290.45426 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.97521 HOMO: -6.20147 LUMO: 0.15238 factor:1 | 1 (-1.15526) | -1 | -1 |
| G: -6290.45426 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.66103 HOMO: -6.43549 LUMO: -0.07075 factor:1 | 1 (-0.84108) | -1 | -1 |
| G: -6290.45426 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.51219 HOMO: -7.02054 LUMO: 0.13061 factor:1 | -1 (0.30776) | -1 | -1 |
| G: -6290.45426 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.43222 HOMO: -7.04503 LUMO: 0.30749 factor:1 | -1 (0.38774) | -1 | -1 |
| G: -6290.45426 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.61187 HOMO: -6.74842 LUMO: -0.99594 factor:1 | -1 (0.20809) | -1 | -1 |
| G: -6290.45426 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.32040 HOMO: -6.35658 LUMO: 0.41633 factor:1 | -1 (0.49955) | -1 | -1 |
| G: -6290.45426 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.59978 HOMO: -6.79740 LUMO: 0.56872 factor:1 | -1 (0.22017) | -1 | -1 |
| G: -6290.45426 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.40179 HOMO: -6.51713 LUMO: -0.05987 factor:1 | 1 (-0.58183) | -1 | -1 |
| G: -6290.45426 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.97271 HOMO: -6.68040 LUMO: 0.34558 factor:1 | 1 (-1.15276) | -1 | -1 |
| G: -6290.45426 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.34627 HOMO: -6.39740 LUMO: 0.50069 factor:1 | 1 (-0.52632) | -1 | -1 |
| G: -6290.45426 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12556.20109 HOMO: -6.91713 LUMO: -0.97145 factor:1 | 1 (-1.38114) | -1 | -1 |
| G: -6290.45426 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.54625 HOMO: -7.10761 LUMO: -0.27483 factor:1 | 1 (-0.72630) | 1 | -1 |
| G: -6290.45426 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.88593 HOMO: -6.98788 LUMO: 0.40273 factor:1 | 1 (-1.06598) | -1 | -1 |
| G: -6290.45426 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.32987 HOMO: -6.87087 LUMO: 0.28572 factor:1 | 1 (-0.50991) | -1 | -1 |
| G: -6290.45426 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.18616 HOMO: -7.36612 LUMO: -0.12245 factor:1 | 1 (-0.36621) | 1 | 1 |
| G: -6290.45426 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.41874 HOMO: -6.72938 LUMO: 0.33742 factor:1 | 1 (-0.59879) | -1 | -1 |
| G: -6290.45426 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.47463 HOMO: -7.32531 LUMO: 0.07619 factor:1 | 1 (-0.65468) | 1 | 1 |
| G: -6290.45426 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.20216 HOMO: -6.87087 LUMO: -0.08436 factor:1 | 1 (-0.38221) | -1 | -1 |
| G: -6290.45426 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.10755 HOMO: -6.67495 LUMO: 0.85988 factor:1 | 1 (-0.28760) | -1 | -1 |
| G: -6290.45426 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.89584 HOMO: -6.96339 LUMO: 0.65307 factor:1 | 1 (-0.07589) | -1 | -1 |
| G: -6290.45426 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.05076 HOMO: -6.58516 LUMO: -0.78641 factor:1 | 1 (-0.23081) | -1 | -1 |
| G: -6290.45426 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.35009 HOMO: -6.56883 LUMO: 0.44355 factor:1 | -1 (0.46986) | -1 | -1 |
| G: -6290.45426 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.53429 HOMO: -6.68312 LUMO: 0.43538 factor:1 | -1 (0.28567) | -1 | -1 |
| G: -6290.45426 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.68240 HOMO: -6.81917 LUMO: 0.20681 factor:1 | -1 (0.13755) | -1 | -1 |
| G: -6290.45426 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.84537 HOMO: -6.91169 LUMO: 0.08163 factor:1 | 1 (-0.02542) | -1 | -1 |
| G: -6290.45426 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.72025 HOMO: -4.88444 LUMO: -0.49253 factor:1 | -1 (0.09970) | -1 | -1 |
| G: -6290.45426 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.33523 HOMO: -6.42189 LUMO: 0.64763 factor:1 | -1 (0.48472) | -1 | -1 |
| G: -6290.45426 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.41393 HOMO: -6.24501 LUMO: 0.55783 factor:1 | -1 (0.40602) | -1 | -1 |
| G: -6290.45426 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.74822 HOMO: -6.41372 LUMO: 0.29388 factor:1 | -1 (0.07173) | -1 | -1 |
| G: -6290.45426 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.38854 HOMO: -5.67902 LUMO: 1.77690 factor:1 | -1 (0.43141) | -1 | -1 |
| G: -6290.45426 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.62724 HOMO: -6.55794 LUMO: 0.05170 factor:1 | -1 (0.19271) | -1 | -1 |
| G: -6290.45426 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.29366 HOMO: -6.52801 LUMO: 0.25851 factor:1 | -1 (0.52630) | -1 | -1 |
| G: -6290.45426 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.77864 HOMO: -7.08857 LUMO: 0.11157 factor:1 | -1 (0.04131) | 1 | 1 |
| G: -6290.45426 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.46397 HOMO: -6.58243 LUMO: 0.75648 factor:1 | -1 (0.35598) | -1 | -1 |
| G: -6290.45426 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.63271 HOMO: -7.22190 LUMO: 0.45171 factor:1 | -1 (0.18724) | 1 | 1 |
| G: -6290.45426 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.62936 HOMO: -6.47087 LUMO: 0.00000 factor:1 | -1 (0.19059) | -1 | -1 |
| G: -6290.45426 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.30228 HOMO: -6.78652 LUMO: 1.32247 factor:1 | -1 (0.51767) | -1 | -1 |
| G: -6290.45426 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.20144 HOMO: -6.74026 LUMO: 1.45309 factor:1 | -1 (0.61851) | -1 | -1 |
| G: -6290.45426 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.38955 HOMO: -6.69944 LUMO: 0.76464 factor:1 | -1 (0.43040) | -1 | -1 |
| G: -6290.45426 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.42691 HOMO: -6.62325 LUMO: 0.64763 factor:1 | -1 (0.39304) | -1 | -1 |
| G: -6290.45426 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.53001 HOMO: -6.45182 LUMO: 0.49253 factor:1 | -1 (0.28994) | -1 | -1 |
| G: -6290.45426 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.44019 HOMO: -7.14843 LUMO: 0.62586 factor:1 | -1 (0.37976) | 1 | 1 |
| G: -6290.45426 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.25118 HOMO: -6.87087 LUMO: 1.53200 factor:1 | -1 (0.56877) | -1 | -1 |
| G: -6290.45426 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.74692 HOMO: -6.54978 LUMO: 0.45171 factor:1 | -1 (0.07304) | -1 | -1 |
| G: -6290.45426 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.66773 HOMO: -6.63686 LUMO: 0.80001 factor:1 | -1 (0.15222) | -1 | -1 |
| G: -6290.45426 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.80055 HOMO: -7.00693 LUMO: 1.56193 factor:1 | -1 (0.01940) | -1 | -1 |
| G: -6290.45426 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.66735 HOMO: -6.02460 LUMO: 1.72792 factor:1 | -1 (0.15260) | -1 | -1 |
| G: -6290.45426 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.41320 HOMO: -6.36746 LUMO: -1.20002 factor:1 | -1 (0.40676) | -1 | -1 |
| G: -6290.45426 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.52378 HOMO: -7.26816 LUMO: -1.06397 factor:1 | -1 (0.29617) | 1 | 1 |
| G: -6290.45426 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.56373 HOMO: -7.34707 LUMO: -1.09662 factor:1 | -1 (0.25622) | 1 | 1 |
| G: -6290.45426 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.19877 HOMO: -7.93212 LUMO: -0.13606 factor:1 | -1 (0.62118) | 1 | 1 |
| G: -6290.45426 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.26500 HOMO: -6.80285 LUMO: 0.58504 factor:1 | -1 (0.55495) | -1 | -1 |
| G: -6290.45426 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.42604 HOMO: -7.12938 LUMO: 0.32926 factor:1 | -1 (0.39391) | 1 | -1 |
| G: -6290.45426 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.46571 HOMO: -6.86815 LUMO: -1.30070 factor:1 | -1 (0.35424) | -1 | -1 |
| G: -6290.45426 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.56142 HOMO: -6.99333 LUMO: -1.03947 factor:1 | -1 (0.25854) | -1 | -1 |
| G: -6290.45426 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.54381 HOMO: -7.56749 LUMO: -0.11157 factor:1 | -1 (0.27614) | 1 | 1 |
| G: -6290.45426 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.67834 HOMO: -7.57293 LUMO: -0.07891 factor:1 | -1 (0.14161) | 1 | 1 |
| G: -6290.45426 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.42332 HOMO: -7.30626 LUMO: 0.27211 factor:1 | -1 (0.39663) | 1 | 1 |
| G: -6290.45426 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.46095 HOMO: -7.77974 LUMO: 0.27211 factor:1 | -1 (0.35900) | 1 | 1 |
| G: -6290.45426 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.10170 HOMO: -7.11578 LUMO: 0.19864 factor:1 | 1 (-0.28175) | 1 | 1 |
| G: -6290.45426 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.20706 HOMO: -7.71171 LUMO: 0.57688 factor:1 | 1 (-0.38711) | 1 | 1 |
| G: -6290.45426 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.30053 HOMO: -7.83688 LUMO: 0.37824 factor:1 | 1 (-0.48058) | 1 | 1 |
| G: -6290.45426 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.34951 HOMO: -6.94979 LUMO: -1.66534 factor:1 | 1 (-0.52956) | -1 | -1 |
| G: -6290.45426 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.98787 HOMO: -6.97156 LUMO: -1.13199 factor:1 | 1 (-0.16792) | -1 | -1 |
| G: -6290.45426 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.99492 HOMO: -6.91441 LUMO: -1.08301 factor:1 | 1 (-0.17497) | -1 | -1 |
| G: -6290.45426 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.35988 HOMO: -6.71849 LUMO: -0.74831 factor:1 | 1 (-0.53993) | -1 | -1 |
| G: -6290.45426 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.15843 HOMO: -7.09401 LUMO: -1.77690 factor:1 | 1 (-0.33848) | -1 | -1 |
| G: -6290.45426 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.70421 HOMO: -6.97156 LUMO: -1.45037 factor:1 | 1 (-0.88426) | -1 | -1 |
| G: -6290.45426 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.80133 HOMO: -7.22462 LUMO: -1.11295 factor:1 | 1 (-0.98138) | 1 | 1 |
| G: -6290.45426 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12556.57601 HOMO: -7.85321 LUMO: 0.16599 factor:1 | 1 (-1.75606) | 1 | 1 |
| G: -6290.45426 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12556.55519 HOMO: -7.71987 LUMO: 0.55511 factor:1 | 1 (-1.73524) | 1 | 1 |
| G: -6290.45426 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.83722 HOMO: -7.63551 LUMO: 0.14422 factor:1 | 1 (-1.01727) | 1 | 1 |
| G: -6290.45426 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12556.40556 HOMO: -6.98788 LUMO: -0.80546 factor:1 | 1 (-1.58561) | -1 | -1 |
| G: -6290.45426 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12556.27206 HOMO: -6.98788 LUMO: -1.16737 factor:1 | 1 (-1.45211) | -1 | -1 |
| G: -6290.45426 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.60386 HOMO: -6.56611 LUMO: -1.60819 factor:1 | 1 (-0.78391) | -1 | -1 |
| G: -6290.45426 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12556.09045 HOMO: -6.95251 LUMO: 0.66396 factor:1 | 1 (-1.27050) | -1 | -1 |
| G: -6290.45426 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.45866 HOMO: -7.35252 LUMO: 0.49797 factor:1 | 1 (-0.63871) | 1 | 1 |
| G: -6290.45426 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.46579 HOMO: -6.90897 LUMO: -0.81090 factor:1 | 1 (-0.64584) | -1 | -1 |
| G: -6290.45426 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.36274 HOMO: -7.04503 LUMO: -1.08301 factor:1 | 1 (-0.54279) | -1 | -1 |
| G: -6290.45426 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.71178 HOMO: -6.92530 LUMO: -1.29526 factor:1 | 1 (-0.89183) | -1 | -1 |
| G: -6290.45426 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.39857 HOMO: -6.93074 LUMO: -1.25444 factor:1 | 1 (-0.57862) | -1 | -1 |
| G: -6290.45426 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.61440 HOMO: -6.73482 LUMO: -0.62042 factor:1 | -1 (0.20555) | -1 | -1 |
| G: -6290.45426 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.61851 HOMO: -7.67633 LUMO: 0.59593 factor:1 | -1 (0.20145) | 1 | 1 |
| G: -6290.45426 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.30334 HOMO: -7.39061 LUMO: -0.19320 factor:1 | -1 (0.51661) | 1 | 1 |
| G: -6290.45426 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.71309 HOMO: -7.55388 LUMO: -0.20136 factor:1 | -1 (0.10686) | 1 | 1 |
| G: -6290.45426 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.50000 HOMO: -7.14027 LUMO: -0.99866 factor:1 | -1 (0.31995) | 1 | 1 |
| G: -6290.45426 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.29050 HOMO: -6.75931 LUMO: -0.73199 factor:1 | -1 (0.52945) | -1 | -1 |
| G: -6290.45426 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.54531 HOMO: -5.45044 LUMO: -0.18776 factor:1 | -1 (0.27464) | -1 | -1 |
| G: -6290.45426 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.39230 HOMO: -6.70761 LUMO: -0.84083 factor:1 | -1 (0.42765) | -1 | -1 |
| G: -6290.45426 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.87047 HOMO: -6.05453 LUMO: -1.06669 factor:1 | 1 (-1.05052) | -1 | -1 |
| G: -6290.45426 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12556.40550 HOMO: -6.86815 LUMO: -0.98233 factor:1 | 1 (-1.58555) | -1 | -1 |
| G: -6290.45426 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.53828 HOMO: -6.73210 LUMO: -0.95240 factor:1 | 1 (-0.71833) | -1 | -1 |
| G: -6290.45426 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12556.52069 HOMO: -5.89671 LUMO: -1.05036 factor:1 | 1 (-1.70074) | -1 | -1 |
| G: -6290.45426 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12556.22874 HOMO: -7.61102 LUMO: 0.33470 factor:1 | 1 (-1.40879) | 1 | 1 |
| G: -6290.45426 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.26968 HOMO: -7.51034 LUMO: 0.23674 factor:1 | -1 (0.55027) | 1 | 1 |
| G: -6290.45426 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.48653 HOMO: -7.41510 LUMO: 0.62858 factor:1 | -1 (0.33342) | 1 | 1 |
| G: -6290.45426 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.27308 HOMO: -6.76203 LUMO: -1.72792 factor:1 | -1 (0.54687) | -1 | -1 |
| G: -6290.45426 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.87967 HOMO: -6.60420 LUMO: -0.45715 factor:1 | 1 (-1.05972) | -1 | -1 |
| G: -6290.45426 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.10967 HOMO: -6.59060 LUMO: -0.58232 factor:1 | 1 (-0.28972) | -1 | -1 |
| G: -6290.45426 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.28453 HOMO: -7.43687 LUMO: -0.76736 factor:1 | 1 (-0.46458) | 1 | 1 |
| G: -6290.45426 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12556.05744 HOMO: -6.08719 LUMO: -0.48708 factor:1 | 1 (-1.23749) | -1 | -1 |
| G: -6290.45426 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.19008 HOMO: -5.88854 LUMO: -0.05714 factor:1 | 1 (-0.37013) | -1 | -1 |
| G: -6290.45426 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.80177 HOMO: -7.34435 LUMO: -0.71838 factor:1 | 1 (-0.98181) | 1 | 1 |
| G: -6290.45426 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.96692 HOMO: -7.46408 LUMO: -0.63130 factor:1 | 1 (-0.14697) | 1 | 1 |
| G: -6290.45426 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.46219 HOMO: -7.00965 LUMO: -1.24900 factor:1 | 1 (-0.64224) | -1 | -1 |
| G: -6290.45426 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.51469 HOMO: -6.91169 LUMO: -0.88981 factor:1 | 1 (-0.69473) | -1 | -1 |
| G: -6290.45426 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.28654 HOMO: -6.78652 LUMO: -0.82178 factor:1 | 1 (-0.46659) | -1 | -1 |
| G: -6290.45426 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.33955 HOMO: -7.80423 LUMO: 0.87076 factor:1 | 1 (-0.51960) | 1 | 1 |
| G: -6290.45426 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.43308 HOMO: -6.97700 LUMO: -1.00954 factor:1 | 1 (-0.61313) | -1 | -1 |
| G: -6290.45426 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.27237 HOMO: -6.92530 LUMO: -0.88165 factor:1 | 1 (-0.45242) | -1 | -1 |
| G: -6290.45426 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.29114 HOMO: -7.14571 LUMO: -1.04492 factor:1 | 1 (-0.47119) | 1 | 1 |
| G: -6290.45426 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.09334 HOMO: -7.49674 LUMO: 0.34558 factor:1 | 1 (-0.27339) | 1 | 1 |
| G: -6290.45426 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.70125 HOMO: -6.44094 LUMO: -1.20819 factor:1 | 1 (-0.88130) | -1 | -1 |
| G: -6290.45426 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.47221 HOMO: -6.47359 LUMO: -1.14016 factor:1 | 1 (-0.65226) | -1 | -1 |
| G: -6290.45426 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.67575 HOMO: -6.61237 LUMO: -0.87076 factor:1 | 1 (-0.85580) | -1 | -1 |
| G: -6290.45426 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12556.24724 HOMO: -6.73754 LUMO: -1.09662 factor:1 | 1 (-1.42729) | -1 | -1 |
| G: -6290.45426 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.42998 HOMO: -6.97700 LUMO: 0.13061 factor:1 | 1 (-0.61002) | -1 | -1 |
| G: -6290.45426 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12556.02416 HOMO: -6.82734 LUMO: 0.59865 factor:1 | 1 (-1.20421) | -1 | -1 |
| G: -6290.45426 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.28502 HOMO: -6.86543 LUMO: -0.91430 factor:1 | 1 (-0.46507) | -1 | -1 |
| G: -6290.45426 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.44636 HOMO: -6.74298 LUMO: 0.28028 factor:1 | 1 (-0.62641) | -1 | -1 |
| G: -6290.45426 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.29955 HOMO: -6.75387 LUMO: 0.19592 factor:1 | 1 (-0.47960) | -1 | -1 |
| G: -6290.45426 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.13996 HOMO: -7.05591 LUMO: 0.10612 factor:1 | 1 (-0.32001) | -1 | -1 |
| G: -6290.45426 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.45069 HOMO: -6.86543 LUMO: 0.49253 factor:1 | -1 (0.36926) | -1 | -1 |
| G: -6290.45426 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.28729 HOMO: -6.11440 LUMO: -1.12655 factor:1 | -1 (0.53266) | -1 | -1 |
| G: -6290.45426 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.28609 HOMO: -6.77291 LUMO: -1.02859 factor:1 | -1 (0.53386) | -1 | -1 |
| G: -6290.45426 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.41619 HOMO: -6.54978 LUMO: 0.29116 factor:1 | -1 (0.40376) | -1 | -1 |
| G: -6290.45426 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.45989 HOMO: -7.18108 LUMO: 0.00000 factor:1 | -1 (0.36006) | 1 | 1 |
| G: -6290.45426 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.17227 HOMO: -6.86271 LUMO: -1.15376 factor:1 | -1 (0.64769) | -1 | -1 |
| G: -6290.45426 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.18378 HOMO: -6.78108 LUMO: -1.22723 factor:1 | -1 (0.63617) | -1 | -1 |
| G: -6290.45426 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.42408 HOMO: -6.40828 LUMO: 0.02449 factor:1 | -1 (0.39587) | -1 | -1 |
| G: -6290.45426 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.23956 HOMO: -6.43821 LUMO: 0.09796 factor:1 | -1 (0.58039) | -1 | -1 |
| G: -6290.45426 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.01452 HOMO: -6.99877 LUMO: 0.40545 factor:1 | -1 (0.80543) | -1 | -1 |
| G: -6290.45426 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.36002 HOMO: -6.68856 LUMO: 0.19320 factor:1 | -1 (0.45993) | -1 | -1 |
| G: -6290.45426 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.24974 HOMO: -7.11034 LUMO: 0.31293 factor:1 | -1 (0.57021) | 1 | 1 |
| G: -6290.45426 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.69458 HOMO: -6.92530 LUMO: -0.85444 factor:1 | 1 (-0.87463) | -1 | -1 |
| G: -6290.45426 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12556.54091 HOMO: -6.60148 LUMO: -0.59865 factor:1 | 1 (-1.72096) | -1 | -1 |
| G: -6290.45426 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.47561 HOMO: -6.72938 LUMO: 0.30749 factor:1 | 1 (-0.65566) | -1 | -1 |
| G: -6290.45426 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.17578 HOMO: -7.31170 LUMO: 0.06803 factor:1 | -1 (0.64418) | 1 | 1 |
| G: -6290.45426 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.32821 HOMO: -7.09129 LUMO: -0.04626 factor:1 | -1 (0.49174) | 1 | 1 |
| G: -6290.45426 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.30291 HOMO: -6.38379 LUMO: -0.76736 factor:1 | -1 (0.51704) | -1 | -1 |
| G: -6290.45426 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.90936 HOMO: -6.13617 LUMO: -0.63947 factor:1 | 1 (-1.08941) | -1 | -1 |
| G: -6290.45426 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.22799 HOMO: -6.92258 LUMO: 0.37007 factor:1 | 1 (-0.40803) | -1 | -1 |
| G: -6290.45426 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.76027 HOMO: -6.35930 LUMO: 0.41361 factor:1 | 1 (-0.94032) | -1 | -1 |
| G: -6290.45426 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.15008 HOMO: -6.60420 LUMO: 0.26667 factor:1 | 1 (-0.33013) | -1 | -1 |
| G: -6290.45426 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.30859 HOMO: -6.04909 LUMO: 1.82588 factor:1 | 1 (-0.48863) | -1 | -1 |
| G: -6290.45426 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12556.02985 HOMO: -6.69672 LUMO: 1.72520 factor:1 | 1 (-1.20990) | -1 | -1 |
| G: -6290.45426 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.39613 HOMO: -6.50080 LUMO: 0.29116 factor:1 | 1 (-0.57617) | -1 | -1 |
| G: -6290.45426 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12556.18607 HOMO: -6.60692 LUMO: -0.43266 factor:1 | 1 (-1.36612) | -1 | -1 |
| G: -6290.45426 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.23756 HOMO: -6.93890 LUMO: 0.39729 factor:1 | 1 (-0.41761) | -1 | -1 |
| G: -6290.45426 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.66379 HOMO: -6.52801 LUMO: -0.47076 factor:1 | -1 (0.15617) | -1 | -1 |
| G: -6290.45426 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.52811 HOMO: -6.41100 LUMO: 0.30477 factor:1 | -1 (0.29184) | -1 | -1 |
| G: -6290.45426 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.71554 HOMO: -6.37291 LUMO: -0.80001 factor:1 | -1 (0.10441) | -1 | -1 |
| G: -6290.45426 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.53162 HOMO: -6.51985 LUMO: 1.44765 factor:1 | -1 (0.28833) | -1 | -1 |
| G: -6290.45426 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.36748 HOMO: -6.64774 LUMO: 0.04626 factor:1 | -1 (0.45247) | -1 | -1 |
| G: -6290.45426 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.70226 HOMO: -6.65863 LUMO: 0.29933 factor:1 | -1 (0.11769) | -1 | -1 |
| G: -6290.45426 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.97987 HOMO: -7.09673 LUMO: 0.28300 factor:1 | 1 (-0.15992) | 1 | 1 |
| G: -6290.45426 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.93024 HOMO: -6.57155 LUMO: -1.11567 factor:1 | 1 (-0.11029) | -1 | -1 |
| G: -6290.45426 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.80942 HOMO: -6.38379 LUMO: -0.60681 factor:1 | -1 (0.01053) | -1 | -1 |
| G: -6290.45426 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.43570 HOMO: -6.60148 LUMO: 0.18232 factor:1 | -1 (0.38425) | -1 | -1 |
| G: -6290.45426 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.96667 HOMO: -6.96067 LUMO: -0.52246 factor:1 | 1 (-0.14672) | -1 | -1 |
| G: -6290.45426 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.70354 HOMO: -6.57427 LUMO: -0.84627 factor:1 | -1 (0.11641) | -1 | -1 |
| G: -6290.45426 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.84681 HOMO: -6.59332 LUMO: -0.98233 factor:1 | 1 (-0.02686) | -1 | -1 |
| G: -6290.45426 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.75056 HOMO: -6.20692 LUMO: -0.27483 factor:1 | -1 (0.06939) | -1 | -1 |
| G: -6290.45426 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.85497 HOMO: -6.81373 LUMO: 0.74559 factor:1 | 1 (-0.03502) | -1 | -1 |
| G: -6290.45426 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.87220 HOMO: -6.60420 LUMO: 0.54695 factor:1 | 1 (-0.05225) | -1 | -1 |
| G: -6290.45426 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.69236 HOMO: -6.58788 LUMO: -0.31021 factor:1 | -1 (0.12759) | -1 | -1 |
| G: -6290.45426 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.53344 HOMO: -6.72938 LUMO: 0.64763 factor:1 | -1 (0.28651) | -1 | -1 |
| G: -6290.45426 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.70104 HOMO: -6.86815 LUMO: 0.32109 factor:1 | -1 (0.11891) | -1 | -1 |
| G: -6290.45426 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.68400 HOMO: -6.63141 LUMO: 0.18776 factor:1 | -1 (0.13595) | -1 | -1 |
| G: -6290.45426 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.37143 HOMO: -7.18653 LUMO: 0.09524 factor:1 | -1 (0.44853) | 1 | 1 |
| G: -6290.45426 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.71546 HOMO: -6.83550 LUMO: 0.03537 factor:1 | -1 (0.10449) | -1 | -1 |
| G: -6290.45426 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.74888 HOMO: -7.47769 LUMO: 0.40817 factor:1 | -1 (0.07108) | 1 | 1 |
| G: -6290.45426 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.37329 HOMO: -6.57971 LUMO: -0.63675 factor:1 | 1 (-0.55334) | -1 | -1 |
| G: -6290.45426 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.41319 HOMO: -6.74842 LUMO: -0.16327 factor:1 | 1 (-0.59324) | -1 | -1 |
| G: -6290.45426 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.61496 HOMO: -7.07224 LUMO: 0.61770 factor:1 | 1 (-0.79501) | 1 | 1 |
| G: -6290.45426 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.59529 HOMO: -6.83006 LUMO: 0.54695 factor:1 | 1 (-0.77533) | -1 | -1 |
| G: -6290.45426 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.52426 HOMO: -6.60148 LUMO: 1.23540 factor:1 | 1 (-0.70431) | -1 | -1 |
| G: -6290.45426 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.46176 HOMO: -6.99061 LUMO: 0.41089 factor:1 | 1 (-0.64181) | -1 | -1 |
| G: -6290.45426 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.80063 HOMO: -6.63686 LUMO: 0.85172 factor:1 | -1 (0.01932) | -1 | -1 |
| G: -6290.45426 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.93165 HOMO: -6.50624 LUMO: 0.12517 factor:1 | 1 (-0.11170) | -1 | -1 |
| G: -6290.45426 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.79171 HOMO: -6.35658 LUMO: 0.36463 factor:1 | -1 (0.02825) | -1 | -1 |
| G: -6290.45426 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.04488 HOMO: -6.34570 LUMO: 0.65035 factor:1 | 1 (-0.22493) | -1 | -1 |
| G: -6290.45426 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.32366 HOMO: -6.63141 LUMO: 1.25717 factor:1 | 1 (-0.50371) | -1 | -1 |
| G: -6290.45426 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.24480 HOMO: -6.91441 LUMO: 1.32792 factor:1 | 1 (-0.42485) | -1 | -1 |
| G: -6290.45426 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.30709 HOMO: -7.15387 LUMO: 0.64219 factor:1 | 1 (-0.48714) | 1 | 1 |
| G: -6290.45426 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.36823 HOMO: -7.17836 LUMO: 0.60409 factor:1 | 1 (-0.54828) | 1 | 1 |
| G: -6290.45426 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.25479 HOMO: -6.92258 LUMO: 0.49525 factor:1 | 1 (-0.43484) | -1 | -1 |
| G: -6290.45426 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.98858 HOMO: -6.31032 LUMO: 0.48708 factor:1 | 1 (-0.16863) | -1 | -1 |
| G: -6290.45426 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.49531 HOMO: -6.49808 LUMO: 0.31021 factor:1 | 1 (-0.67536) | -1 | -1 |
| G: -6290.45426 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.42979 HOMO: -6.48447 LUMO: 0.37552 factor:1 | 1 (-0.60983) | -1 | -1 |
| G: -6290.45426 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.28491 HOMO: -6.66135 LUMO: -1.08301 factor:1 | 1 (-0.46496) | -1 | -1 |
| G: -6290.45426 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.09043 HOMO: -6.33481 LUMO: -0.51974 factor:1 | 1 (-0.27048) | -1 | -1 |
| G: -6290.45426 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.10589 HOMO: -6.76475 LUMO: -0.15238 factor:1 | 1 (-0.28594) | -1 | -1 |
| G: -6290.45426 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.33610 HOMO: -6.93346 LUMO: -0.10885 factor:1 | 1 (-0.51615) | -1 | -1 |
| G: -6290.45426 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.36807 HOMO: -7.19741 LUMO: 0.73199 factor:1 | 1 (-0.54812) | 1 | 1 |
| G: -6290.45426 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.10679 HOMO: -6.82734 LUMO: 0.88437 factor:1 | 1 (-0.28684) | -1 | -1 |
| G: -6290.45426 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.94224 HOMO: -7.01237 LUMO: 0.02721 factor:1 | 1 (-0.12229) | -1 | -1 |
| G: -6290.45426 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.29370 HOMO: -6.39195 LUMO: 1.46941 factor:1 | 1 (-0.47375) | -1 | -1 |
| G: -6290.45426 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.35142 HOMO: -6.53890 LUMO: 1.32792 factor:1 | 1 (-0.53147) | -1 | -1 |
| G: -6290.45426 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.63042 HOMO: -6.82734 LUMO: 1.98099 factor:1 | -1 (0.18953) | -1 | -1 |
| G: -6290.45426 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.56806 HOMO: -6.74570 LUMO: 1.68983 factor:1 | -1 (0.25190) | -1 | -1 |
| G: -6290.45426 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.39341 HOMO: -6.41100 LUMO: 1.39050 factor:1 | -1 (0.42654) | -1 | -1 |
| G: -6290.45426 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.21458 HOMO: -5.92664 LUMO: 1.65989 factor:1 | -1 (0.60537) | -1 | -1 |
| G: -6290.45426 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.14043 HOMO: -6.07630 LUMO: 1.54833 factor:1 | -1 (0.67952) | -1 | -1 |
| G: -6290.45426 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.77296 HOMO: -6.45998 LUMO: 0.68573 factor:1 | -1 (0.04699) | -1 | -1 |
| G: -6290.45426 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.45850 HOMO: -6.52801 LUMO: 0.41361 factor:1 | -1 (0.36145) | -1 | -1 |
| G: -6290.45426 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.61687 HOMO: -6.77564 LUMO: 0.42178 factor:1 | -1 (0.20308) | -1 | -1 |
| G: -6290.45426 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.70006 HOMO: -6.56339 LUMO: 1.65717 factor:1 | -1 (0.11989) | -1 | -1 |
| G: -6290.45426 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.50748 HOMO: -5.85861 LUMO: 1.90752 factor:1 | -1 (0.31247) | -1 | -1 |
| G: -6290.45426 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.34389 HOMO: -6.77019 LUMO: -2.48440 factor:1 | -1 (0.47606) | -1 | -1 |
| G: -6290.45426 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.59108 HOMO: -6.53890 LUMO: -1.82588 factor:1 | -1 (0.22887) | -1 | -1 |
| G: -6290.45426 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.49173 HOMO: -6.50352 LUMO: -1.66806 factor:1 | -1 (0.32822) | -1 | -1 |
| G: -6290.45426 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.62348 HOMO: -6.90625 LUMO: 0.43538 factor:1 | -1 (0.19647) | -1 | -1 |
| G: -6290.45426 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.41907 HOMO: -6.85455 LUMO: 0.53062 factor:1 | -1 (0.40088) | -1 | -1 |
| G: -6290.45426 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.27417 HOMO: -6.49536 LUMO: 0.31021 factor:1 | -1 (0.54578) | -1 | -1 |
| G: -6290.45426 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.55823 HOMO: -4.97696 LUMO: -0.09252 factor:1 | -1 (0.26172) | -1 | -1 |
| G: -6290.45426 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.24412 HOMO: -5.31166 LUMO: 0.34286 factor:1 | 1 (-0.42417) | -1 | -1 |
| G: -6290.45426 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.28050 HOMO: -6.42461 LUMO: 0.74287 factor:1 | 1 (-0.46055) | -1 | -1 |
| G: -6290.45426 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.20548 HOMO: -6.59604 LUMO: 0.62858 factor:1 | 1 (-0.38553) | -1 | -1 |
| G: -6290.45426 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.85255 HOMO: -6.45998 LUMO: -0.61770 factor:1 | 1 (-0.03260) | -1 | -1 |
| G: -6290.45426 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.27327 HOMO: -6.75659 LUMO: -0.34014 factor:1 | 1 (-0.45331) | -1 | -1 |
| G: -6290.45426 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.07533 HOMO: -6.63958 LUMO: 0.36191 factor:1 | 1 (-0.25538) | -1 | -1 |
| G: -6290.45426 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.75056 HOMO: -5.92936 LUMO: -0.67484 factor:1 | -1 (0.06939) | -1 | -1 |
| G: -6290.45426 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.52359 HOMO: -5.67630 LUMO: 1.80956 factor:1 | -1 (0.29636) | -1 | -1 |
| G: -6290.45426 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.60291 HOMO: -6.50352 LUMO: -0.78369 factor:1 | -1 (0.21704) | -1 | -1 |
| G: -6290.45426 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.25371 HOMO: -6.35930 LUMO: -0.75648 factor:1 | -1 (0.56624) | -1 | -1 |
| G: -6290.45426 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.67540 HOMO: -6.74298 LUMO: 0.48980 factor:1 | -1 (0.14455) | -1 | -1 |
| G: -6290.45426 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.34794 HOMO: -6.85183 LUMO: 0.15510 factor:1 | -1 (0.47201) | -1 | -1 |
| G: -6290.45426 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.19618 HOMO: -6.90897 LUMO: 0.26123 factor:1 | -1 (0.62377) | -1 | -1 |
| G: -6290.45426 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.47156 HOMO: -6.85999 LUMO: 0.47892 factor:1 | -1 (0.34839) | -1 | -1 |
| G: -6290.45426 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.44552 HOMO: -6.69944 LUMO: 0.57416 factor:1 | -1 (0.37443) | -1 | -1 |
| G: -6290.45426 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.63059 HOMO: -6.74026 LUMO: 0.69933 factor:1 | -1 (0.18936) | -1 | -1 |
| G: -6290.45426 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.74634 HOMO: -6.52801 LUMO: 0.75376 factor:1 | -1 (0.07361) | -1 | -1 |
| G: -6290.45426 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.83247 HOMO: -7.05863 LUMO: 0.44627 factor:1 | 1 (-0.01252) | -1 | -1 |
| G: -6290.45426 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.58528 HOMO: -6.96339 LUMO: 0.48164 factor:1 | -1 (0.23467) | -1 | -1 |
| G: -6290.45426 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.54672 HOMO: -6.95795 LUMO: 0.44355 factor:1 | -1 (0.27323) | -1 | -1 |
| G: -6290.45426 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.42247 HOMO: -6.36746 LUMO: 0.58777 factor:1 | -1 (0.39748) | -1 | -1 |
| G: -6290.45426 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.54158 HOMO: -6.69400 LUMO: 0.40545 factor:1 | -1 (0.27837) | -1 | -1 |
| G: -6290.45426 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.55548 HOMO: -6.30760 LUMO: -0.66668 factor:1 | -1 (0.26447) | -1 | -1 |
| G: -6290.45426 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.29717 HOMO: -6.53617 LUMO: -0.64491 factor:1 | -1 (0.52279) | -1 | -1 |
| G: -6290.45426 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.61508 HOMO: -6.80829 LUMO: 0.17415 factor:1 | -1 (0.20487) | -1 | -1 |
| G: -6290.45426 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.26838 HOMO: -6.80285 LUMO: 0.73471 factor:1 | -1 (0.55157) | -1 | -1 |
| G: -6290.45426 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.37134 HOMO: -6.43821 LUMO: 0.21769 factor:1 | -1 (0.44861) | -1 | -1 |
| G: -6290.45426 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.18625 HOMO: -6.98788 LUMO: 0.10885 factor:1 | -1 (0.63370) | -1 | -1 |
| G: -6290.45426 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.00451 HOMO: -7.15115 LUMO: 0.40817 factor:1 | -1 (0.81544) | 1 | 1 |
| G: -6290.45426 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.50678 HOMO: -6.00011 LUMO: -0.98505 factor:1 | -1 (0.31318) | -1 | -1 |
| G: -6290.45426 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.17507 HOMO: -6.16882 LUMO: -0.77825 factor:1 | -1 (0.64488) | -1 | -1 |
| G: -6290.45426 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.76575 HOMO: -6.30760 LUMO: 0.34831 factor:1 | -1 (0.05421) | -1 | -1 |
| G: -6290.45426 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.65780 HOMO: -6.64502 LUMO: 0.63403 factor:1 | -1 (0.16215) | -1 | -1 |
| G: -6290.45426 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.14975 HOMO: -6.93618 LUMO: 0.96600 factor:1 | 1 (-0.32980) | -1 | -1 |
| G: -6290.45426 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.18023 HOMO: -6.45182 LUMO: 0.16327 factor:1 | 1 (-0.36028) | -1 | -1 |
| G: -6290.45426 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.04140 HOMO: -6.99605 LUMO: 0.20953 factor:1 | 1 (-0.22145) | -1 | -1 |
| G: -6290.45426 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.36113 HOMO: -6.72665 LUMO: 0.32654 factor:1 | 1 (-0.54118) | -1 | -1 |
| G: -6290.45426 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.41039 HOMO: -6.38379 LUMO: 0.45443 factor:1 | -1 (0.40956) | -1 | -1 |
| G: -6290.45426 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.26166 HOMO: -6.65318 LUMO: 0.04354 factor:1 | -1 (0.55830) | -1 | -1 |
| G: -6290.45426 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12553.97194 HOMO: -6.94707 LUMO: -1.68438 factor:1 | -1 (0.84802) | -1 | -1 |
| G: -6290.45426 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.07330 HOMO: -6.71849 LUMO: 0.15783 factor:1 | -1 (0.74665) | -1 | -1 |
| G: -6290.45426 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12553.76902 HOMO: -6.97156 LUMO: 0.43266 factor:1 | -1 (1.05093) | -1 | -1 |
| G: -6290.45426 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12553.41067 HOMO: -6.91441 LUMO: -0.54695 factor:1 | -1 (1.40928) | -1 | -1 |
| G: -6290.45426 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.17548 HOMO: -6.74842 LUMO: -0.76192 factor:1 | -1 (0.64447) | -1 | -1 |
| G: -6290.45426 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.85171 HOMO: -6.70489 LUMO: 0.19048 factor:1 | 1 (-0.03176) | -1 | -1 |
| G: -6290.45426 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.72523 HOMO: -7.25728 LUMO: 0.33470 factor:1 | -1 (0.09472) | 1 | -1 |
| G: -6290.45426 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.63233 HOMO: -6.96339 LUMO: 0.55511 factor:1 | -1 (0.18762) | -1 | -1 |
| G: -6290.45426 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.82349 HOMO: -6.77564 LUMO: 0.72382 factor:1 | 1 (-0.00354) | -1 | -1 |
| G: -6290.45426 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.54321 HOMO: -6.75387 LUMO: 0.39729 factor:1 | -1 (0.27674) | -1 | -1 |
| G: -6290.45426 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.64433 HOMO: -7.00149 LUMO: 0.06531 factor:1 | -1 (0.17562) | -1 | -1 |
| G: -6290.45426 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.39890 HOMO: -7.09945 LUMO: 0.33470 factor:1 | 1 (-0.57895) | 1 | 1 |
| G: -6290.45426 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.51724 HOMO: -7.20830 LUMO: 0.59593 factor:1 | 1 (-0.69729) | 1 | 1 |
| G: -6290.45426 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.55733 HOMO: -6.40556 LUMO: 0.56600 factor:1 | 1 (-0.73737) | -1 | -1 |
| G: -6290.45426 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.30592 HOMO: -6.77291 LUMO: 0.73471 factor:1 | 1 (-0.48597) | -1 | -1 |
| G: -6290.45426 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.35501 HOMO: -6.65046 LUMO: 0.09796 factor:1 | 1 (-0.53506) | -1 | -1 |
| G: -6290.45426 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.73402 HOMO: -6.95795 LUMO: 0.22313 factor:1 | -1 (0.08593) | -1 | -1 |
| G: -6290.45426 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.80036 HOMO: -6.85727 LUMO: 0.04626 factor:1 | -1 (0.01959) | -1 | -1 |
| G: -6290.45426 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.63363 HOMO: -7.27360 LUMO: 0.42178 factor:1 | -1 (0.18632) | 1 | 1 |
| G: -6290.45426 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.52204 HOMO: -6.78924 LUMO: -0.13334 factor:1 | -1 (0.29791) | -1 | -1 |
| G: -6290.45426 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.42841 HOMO: -6.63141 LUMO: 0.38368 factor:1 | -1 (0.39154) | -1 | -1 |
| G: -6290.45426 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.35205 HOMO: -6.92258 LUMO: 0.39184 factor:1 | -1 (0.46790) | -1 | -1 |
| G: -6290.45426 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.38996 HOMO: -6.19331 LUMO: -0.46804 factor:1 | -1 (0.42999) | -1 | -1 |
| G: -6290.45426 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.11594 HOMO: -7.26544 LUMO: -0.05442 factor:1 | -1 (0.70401) | 1 | 1 |
| G: -6290.45426 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.48307 HOMO: -7.09401 LUMO: 0.30749 factor:1 | -1 (0.33688) | 1 | 1 |
| G: -6290.45426 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.35400 HOMO: -6.14705 LUMO: -0.88709 factor:1 | 1 (-0.53405) | -1 | -1 |
| G: -6290.45426 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.54952 HOMO: -6.53617 LUMO: -0.28572 factor:1 | 1 (-0.72956) | -1 | -1 |
| G: -6290.45426 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.08924 HOMO: -6.37291 LUMO: -0.67212 factor:1 | 1 (-0.26928) | -1 | -1 |
| G: -6290.45426 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.51860 HOMO: -6.65591 LUMO: 0.03810 factor:1 | 1 (-0.69865) | -1 | -1 |
| G: -6290.45426 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.36355 HOMO: -7.11034 LUMO: 0.75103 factor:1 | 1 (-0.54360) | 1 | 1 |
| G: -6290.45426 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.80575 HOMO: -6.85183 LUMO: -0.05987 factor:1 | -1 (0.01420) | -1 | -1 |
| G: -6290.45426 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.54626 HOMO: -6.70761 LUMO: -0.05442 factor:1 | -1 (0.27369) | -1 | -1 |
| G: -6290.45426 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.68245 HOMO: -6.23413 LUMO: 0.06259 factor:1 | -1 (0.13750) | -1 | -1 |
| G: -6290.45426 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.37311 HOMO: -6.55794 LUMO: 0.74015 factor:1 | -1 (0.44684) | -1 | -1 |
| G: -6290.45426 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.17839 HOMO: -7.27905 LUMO: 0.26939 factor:1 | -1 (0.64156) | 1 | 1 |
| G: -6290.45426 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.39826 HOMO: -6.34842 LUMO: -0.86804 factor:1 | -1 (0.42169) | -1 | -1 |
| G: -6290.45426 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.60539 HOMO: -6.27222 LUMO: 1.46125 factor:1 | -1 (0.21456) | -1 | -1 |
| G: -6290.45426 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.75625 HOMO: -6.65046 LUMO: 2.04902 factor:1 | -1 (0.06370) | -1 | -1 |
| G: -6290.45426 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.44792 HOMO: -7.11850 LUMO: -1.14016 factor:1 | -1 (0.37203) | 1 | -1 |
| G: -6290.45426 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.55932 HOMO: -6.88720 LUMO: -1.20274 factor:1 | -1 (0.26063) | -1 | -1 |
| G: -6290.45426 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.62261 HOMO: -6.69400 LUMO: -0.31565 factor:1 | -1 (0.19734) | -1 | -1 |
| G: -6290.45426 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.19605 HOMO: -6.95523 LUMO: -1.55377 factor:1 | -1 (0.62390) | -1 | -1 |
| G: -6290.45426 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.19891 HOMO: -6.41372 LUMO: -0.83539 factor:1 | -1 (0.62105) | -1 | -1 |
| G: -6290.45426 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12553.93044 HOMO: -6.13889 LUMO: -0.90070 factor:1 | -1 (0.88951) | -1 | -1 |
| G: -6290.45426 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.33929 HOMO: -6.44366 LUMO: -0.55511 factor:1 | -1 (0.48066) | -1 | -1 |
| G: -6290.45426 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.55102 HOMO: -6.10079 LUMO: -0.71022 factor:1 | -1 (0.26893) | -1 | -1 |
| G: -6290.45426 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.54346 HOMO: -6.90353 LUMO: -0.64763 factor:1 | -1 (0.27649) | -1 | -1 |
| G: -6290.45426 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.52451 HOMO: -6.65046 LUMO: -0.82450 factor:1 | 1 (-0.70456) | -1 | -1 |
| G: -6290.45426 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.58799 HOMO: -6.81645 LUMO: -0.85444 factor:1 | 1 (-0.76804) | -1 | -1 |
| G: -6290.45426 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.34230 HOMO: -6.20692 LUMO: 1.30887 factor:1 | 1 (-0.52235) | -1 | -1 |
| G: -6290.45426 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.37732 HOMO: -5.96201 LUMO: 1.33880 factor:1 | 1 (-0.55737) | -1 | -1 |
| G: -6290.45426 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.20799 HOMO: -6.52529 LUMO: 1.58914 factor:1 | 1 (-0.38803) | -1 | -1 |
| G: -6290.45426 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.24102 HOMO: -6.58516 LUMO: 1.97555 factor:1 | 1 (-0.42107) | -1 | -1 |
| G: -6290.45426 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.19558 HOMO: -6.84366 LUMO: 0.15783 factor:1 | 1 (-0.37563) | -1 | -1 |
| G: -6290.45426 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.38140 HOMO: -6.45726 LUMO: 0.42994 factor:1 | 1 (-0.56145) | -1 | -1 |
| G: -6290.45426 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.28284 HOMO: -6.75387 LUMO: 0.14422 factor:1 | 1 (-0.46289) | -1 | -1 |
| G: -6290.45426 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.01748 HOMO: -6.69944 LUMO: 1.79051 factor:1 | 1 (-0.19753) | -1 | -1 |
| G: -6290.45426 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.35865 HOMO: -6.59876 LUMO: 1.90208 factor:1 | 1 (-0.53870) | -1 | -1 |
| G: -6290.45426 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.25729 HOMO: -7.05863 LUMO: 1.20819 factor:1 | 1 (-0.43734) | -1 | -1 |
| G: -6290.45426 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.27884 HOMO: -6.54978 LUMO: 2.01636 factor:1 | 1 (-0.45889) | -1 | -1 |
| G: -6290.45426 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.10858 HOMO: -5.52119 LUMO: 1.95106 factor:1 | 1 (-0.28863) | -1 | -1 |
| G: -6290.45426 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.32355 HOMO: -6.53617 LUMO: 1.60275 factor:1 | 1 (-0.50360) | -1 | -1 |
| G: -6290.45426 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.35972 HOMO: -6.11440 LUMO: 1.89119 factor:1 | 1 (-0.53977) | -1 | -1 |
| G: -6290.45426 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.51466 HOMO: -7.31986 LUMO: 0.48708 factor:1 | 1 (-0.69471) | 1 | 1 |
| G: -6290.45426 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.34935 HOMO: -6.76475 LUMO: -0.75648 factor:1 | 1 (-0.52940) | -1 | -1 |
| G: -6290.45426 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.16924 HOMO: -6.76747 LUMO: -1.06941 factor:1 | 1 (-0.34929) | -1 | -1 |
| G: -6290.45426 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.10091 HOMO: -6.87087 LUMO: 0.72927 factor:1 | 1 (-0.28096) | -1 | -1 |
| G: -6290.45426 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.39294 HOMO: -7.00965 LUMO: 0.02177 factor:1 | 1 (-0.57299) | -1 | -1 |
| G: -6290.45426 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.40271 HOMO: -6.54706 LUMO: -0.03265 factor:1 | 1 (-0.58276) | -1 | -1 |
| G: -6290.45426 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.43825 HOMO: -6.62325 LUMO: -0.63675 factor:1 | 1 (-0.61830) | -1 | -1 |
| G: -6290.45426 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.23220 HOMO: -7.03414 LUMO: -1.24084 factor:1 | 1 (-0.41225) | -1 | -1 |
| G: -6290.45426 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.40211 HOMO: -7.04503 LUMO: -0.10068 factor:1 | 1 (-0.58216) | -1 | -1 |
| G: -6290.45426 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.02986 HOMO: -6.67223 LUMO: 0.03537 factor:1 | 1 (-0.20991) | -1 | -1 |
| G: -6290.45426 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.99214 HOMO: -6.82734 LUMO: 0.58777 factor:1 | 1 (-0.17219) | -1 | -1 |
| G: -6290.45426 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.32070 HOMO: -6.84366 LUMO: 0.46531 factor:1 | 1 (-0.50074) | -1 | -1 |
| G: -6290.45426 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.17234 HOMO: -7.03959 LUMO: -1.15104 factor:1 | 1 (-0.35239) | -1 | -1 |
| G: -6290.45426 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.45336 HOMO: -6.91169 LUMO: -0.41361 factor:1 | -1 (0.36659) | -1 | -1 |
| G: -6290.45426 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.56604 HOMO: -7.10217 LUMO: -0.44627 factor:1 | -1 (0.25391) | 1 | 1 |
| G: -6290.45426 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.59407 HOMO: -6.88176 LUMO: -0.19592 factor:1 | -1 (0.22588) | -1 | -1 |
| G: -6290.45426 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.70833 HOMO: -7.21374 LUMO: -0.46531 factor:1 | -1 (0.11162) | 1 | 1 |
| G: -6290.45426 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.32947 HOMO: -6.54978 LUMO: 0.16871 factor:1 | -1 (0.49049) | -1 | -1 |
| G: -6290.45426 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.38666 HOMO: -6.71305 LUMO: -0.13061 factor:1 | -1 (0.43329) | -1 | -1 |
| G: -6290.45426 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.43706 HOMO: -6.74842 LUMO: -0.36191 factor:1 | -1 (0.38289) | -1 | -1 |
| G: -6290.45426 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.62566 HOMO: -6.74570 LUMO: -0.09796 factor:1 | -1 (0.19429) | -1 | -1 |
| G: -6290.45426 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.51948 HOMO: -6.93890 LUMO: -0.27211 factor:1 | -1 (0.30047) | -1 | -1 |
| G: -6290.45426 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.48922 HOMO: -6.88720 LUMO: -0.18776 factor:1 | -1 (0.33073) | -1 | -1 |
| G: -6290.45426 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.33834 HOMO: -6.74842 LUMO: 0.02993 factor:1 | -1 (0.48161) | -1 | -1 |
| G: -6290.45426 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.45330 HOMO: -6.70216 LUMO: 0.01361 factor:1 | 1 (-0.63335) | -1 | -1 |
| G: -6290.45426 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.46927 HOMO: -6.90625 LUMO: 0.00544 factor:1 | 1 (-0.64932) | -1 | -1 |
| G: -6290.45426 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.21560 HOMO: -6.18243 LUMO: 0.25851 factor:1 | 1 (-0.39565) | -1 | -1 |
| G: -6290.45426 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.54524 HOMO: -6.32937 LUMO: -0.20953 factor:1 | 1 (-0.72529) | -1 | -1 |
| G: -6290.45426 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.30859 HOMO: -6.78108 LUMO: 0.00544 factor:1 | 1 (-0.48863) | -1 | -1 |
| G: -6290.45426 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.15718 HOMO: -5.97562 LUMO: 0.28572 factor:1 | 1 (-0.33723) | -1 | -1 |
| G: -6290.45426 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.97383 HOMO: -5.97290 LUMO: -0.18504 factor:1 | 1 (-0.15388) | -1 | -1 |
| G: -6290.45426 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.38042 HOMO: -6.12800 LUMO: 0.42178 factor:1 | 1 (-0.56047) | -1 | -1 |
| G: -6290.45426 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.17073 HOMO: -6.24229 LUMO: -0.00816 factor:1 | 1 (-0.35078) | -1 | -1 |
| G: -6290.45426 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.34355 HOMO: -6.61781 LUMO: 0.12789 factor:1 | 1 (-0.52360) | -1 | -1 |
| G: -6290.45426 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.29865 HOMO: -6.70489 LUMO: 0.14694 factor:1 | 1 (-0.47870) | -1 | -1 |
| G: -6290.45426 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.10551 HOMO: -6.86543 LUMO: -0.21225 factor:1 | 1 (-0.28556) | -1 | -1 |
| G: -6290.45426 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.00766 HOMO: -6.90081 LUMO: -0.20136 factor:1 | 1 (-0.18770) | -1 | -1 |
| G: -6290.45426 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.39501 HOMO: -7.12938 LUMO: -0.25851 factor:1 | 1 (-0.57506) | 1 | 1 |
| G: -6290.45426 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.25174 HOMO: -6.93074 LUMO: -0.26667 factor:1 | 1 (-0.43179) | -1 | -1 |
| G: -6290.45426 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.95043 HOMO: -7.00421 LUMO: -0.31021 factor:1 | 1 (-0.13048) | -1 | -1 |
| G: -6290.45426 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.90599 HOMO: -7.10761 LUMO: -0.17415 factor:1 | 1 (-0.08604) | 1 | 1 |
| G: -6290.45426 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.79331 HOMO: -8.21240 LUMO: 0.05987 factor:1 | -1 (0.02664) | 1 | 1 |
| G: -6290.45426 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.46476 HOMO: -7.14843 LUMO: -0.46531 factor:1 | -1 (0.35519) | 1 | -1 |
| G: -6290.45426 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.19547 HOMO: -6.80829 LUMO: -0.29933 factor:1 | 1 (-0.37552) | -1 | -1 |
| G: -6290.45426 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.06020 HOMO: -6.84094 LUMO: -0.53606 factor:1 | 1 (-0.24025) | -1 | -1 |
| G: -6290.45426 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.85639 HOMO: -6.81917 LUMO: -0.26667 factor:1 | 1 (-0.03644) | -1 | -1 |
| G: -6290.45426 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.24048 HOMO: -6.85727 LUMO: -1.20002 factor:1 | 1 (-0.42052) | -1 | -1 |
| G: -6290.45426 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.06317 HOMO: -6.39468 LUMO: -1.06941 factor:1 | 1 (-0.24322) | -1 | -1 |
| G: -6290.45426 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.20154 HOMO: -6.00827 LUMO: -1.94017 factor:1 | 1 (-0.38159) | -1 | -1 |
| G: -6290.45426 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.41819 HOMO: -6.80829 LUMO: 0.18504 factor:1 | 1 (-0.59824) | -1 | -1 |
| G: -6290.45426 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.97078 HOMO: -6.54434 LUMO: -0.95784 factor:1 | 1 (-0.15083) | -1 | -1 |
| G: -6290.45426 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.90708 HOMO: -6.45454 LUMO: -0.07347 factor:1 | 1 (-0.08713) | -1 | -1 |
| G: -6290.45426 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.99133 HOMO: -5.33887 LUMO: 1.11839 factor:1 | 1 (-0.17138) | -1 | -1 |
| G: -6290.45426 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.35686 HOMO: -5.75249 LUMO: 0.70477 factor:1 | 1 (-0.53691) | -1 | -1 |
| G: -6290.45426 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.15615 HOMO: -5.64092 LUMO: 0.87076 factor:1 | 1 (-0.33620) | -1 | -1 |
| G: -6290.45426 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.22790 HOMO: -5.14295 LUMO: 1.06124 factor:1 | 1 (-0.40795) | -1 | -1 |
| G: -6290.45426 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.13960 HOMO: -5.05043 LUMO: 1.21091 factor:1 | 1 (-0.31965) | -1 | -1 |
| G: -6290.45426 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.36355 HOMO: -5.05588 LUMO: 1.02859 factor:1 | 1 (-0.54360) | -1 | -1 |
| G: -6290.45426 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.86058 HOMO: -5.76337 LUMO: 0.79457 factor:1 | 1 (-0.04063) | -1 | -1 |
| G: -6290.45426 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.73361 HOMO: -5.01506 LUMO: 1.00138 factor:1 | -1 (0.08634) | -1 | -1 |
| G: -6290.45426 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.83489 HOMO: -4.84363 LUMO: 1.53744 factor:1 | 1 (-0.01494) | -1 | -1 |
| G: -6290.45426 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.46999 HOMO: -5.17833 LUMO: 1.45309 factor:1 | -1 (0.34997) | -1 | -1 |
| G: -6290.45426 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.11628 HOMO: -5.13751 LUMO: 0.51157 factor:1 | 1 (-0.29633) | -1 | -1 |
| G: -6290.45426 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.91271 HOMO: -5.56473 LUMO: 0.32109 factor:1 | 1 (-0.09276) | -1 | -1 |
| G: -6290.45426 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.90833 HOMO: -4.69941 LUMO: 1.14016 factor:1 | 1 (-0.08838) | -1 | -1 |
| G: -6290.45426 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.82675 HOMO: -4.49260 LUMO: 1.86398 factor:1 | 1 (-0.00680) | -1 | -1 |
| G: -6290.45426 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.64019 HOMO: -4.32117 LUMO: 1.68438 factor:1 | -1 (0.17976) | -1 | -1 |
| G: -6290.45426 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.11182 HOMO: -4.44906 LUMO: 1.37690 factor:1 | 1 (-0.29187) | -1 | -1 |
| G: -6290.45426 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.80557 HOMO: -4.62049 LUMO: 1.34968 factor:1 | 1 (-0.98562) | -1 | -1 |
| G: -6290.45426 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12556.58268 HOMO: -4.59600 LUMO: 1.58370 factor:1 | 1 (-1.76273) | -1 | -1 |
| G: -6290.45426 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.45983 HOMO: -4.98785 LUMO: 1.46669 factor:1 | 1 (-0.63988) | -1 | -1 |
| G: -6290.45426 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.60160 HOMO: -5.06676 LUMO: 1.27349 factor:1 | 1 (-0.78165) | -1 | -1 |
| G: -6290.45426 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.80664 HOMO: -5.09125 LUMO: 1.13471 factor:1 | 1 (-0.98668) | -1 | -1 |
| G: -6290.45426 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.39713 HOMO: -4.84635 LUMO: 1.33608 factor:1 | 1 (-0.57718) | -1 | -1 |
| G: -6290.45426 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.89643 HOMO: -4.94431 LUMO: 1.18370 factor:1 | 1 (-1.07648) | -1 | -1 |
| G: -6290.45426 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12556.40423 HOMO: -4.92526 LUMO: 1.39867 factor:1 | 1 (-1.58427) | -1 | -1 |
| G: -6290.45426 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12556.12193 HOMO: -5.71983 LUMO: 0.60137 factor:1 | 1 (-1.30198) | -1 | -1 |
| G: -6290.45426 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12556.58015 HOMO: -5.10486 LUMO: 1.05580 factor:1 | 1 (-1.76020) | -1 | -1 |
| G: -6290.45426 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.42173 HOMO: -5.20282 LUMO: 1.01226 factor:1 | 1 (-0.60178) | -1 | -1 |
| G: -6290.45426 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.23816 HOMO: -4.98513 LUMO: 1.53744 factor:1 | 1 (-0.41821) | -1 | -1 |
| G: -6290.45426 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.05566 HOMO: -5.67085 LUMO: 0.17687 factor:1 | 1 (-0.23571) | -1 | -1 |
| G: -6290.45426 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12556.52153 HOMO: -5.87222 LUMO: 0.12517 factor:1 | 1 (-1.70158) | -1 | -1 |
| G: -6290.45426 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.73961 HOMO: -5.20826 LUMO: 0.91702 factor:1 | 1 (-0.91966) | -1 | -1 |
| G: -6290.45426 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12556.66714 HOMO: -5.94569 LUMO: 0.63130 factor:1 | 1 (-1.84719) | -1 | -1 |
| G: -6290.45426 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.36274 HOMO: -5.35792 LUMO: 0.91430 factor:1 | 1 (-0.54279) | -1 | -1 |
| G: -6290.45426 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12556.13257 HOMO: -5.36336 LUMO: 1.44220 factor:1 | 1 (-1.31262) | -1 | -1 |
| G: -6290.45426 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.88773 HOMO: -5.83412 LUMO: 0.71294 factor:1 | 1 (-1.06777) | -1 | -1 |
| G: -6290.45426 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.67365 HOMO: -4.97696 LUMO: 1.72792 factor:1 | 1 (-0.85370) | -1 | -1 |
| G: -6290.45426 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.52623 HOMO: -5.55929 LUMO: 0.23130 factor:1 | -1 (0.29372) | -1 | -1 |
| G: -6290.45426 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.39515 HOMO: -5.71167 LUMO: 0.47348 factor:1 | -1 (0.42480) | -1 | -1 |
| G: -6290.45426 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.93986 HOMO: -7.31986 LUMO: -2.54699 factor:1 | 1 (-1.11991) | -1 | -1 |
| G: -6290.45426 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.39808 HOMO: -5.34704 LUMO: 1.19730 factor:1 | 1 (-0.57813) | -1 | -1 |
| G: -6290.45426 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.79034 HOMO: -5.45860 LUMO: 0.80818 factor:1 | 1 (-0.97039) | -1 | -1 |
| G: -6290.45426 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.34219 HOMO: -5.12663 LUMO: 1.20274 factor:1 | 1 (-0.52224) | -1 | -1 |
| G: -6290.45426 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.28611 HOMO: -5.37153 LUMO: 1.05580 factor:1 | 1 (-0.46616) | -1 | -1 |
| G: -6290.45426 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.39599 HOMO: -5.47221 LUMO: 0.97961 factor:1 | 1 (-0.57604) | -1 | -1 |
| G: -6290.45426 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.31789 HOMO: -5.06948 LUMO: 1.12111 factor:1 | 1 (-0.49794) | -1 | -1 |
| G: -6290.45426 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.45928 HOMO: -5.19737 LUMO: 1.25444 factor:1 | 1 (-0.63933) | -1 | -1 |
| G: -6290.45426 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.24505 HOMO: -5.27901 LUMO: 1.00682 factor:1 | 1 (-0.42510) | -1 | -1 |
| G: -6290.45426 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.11258 HOMO: -5.38513 LUMO: 0.49253 factor:1 | 1 (-0.29263) | -1 | -1 |
| G: -6290.45426 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.18151 HOMO: -5.12390 LUMO: 1.22995 factor:1 | 1 (-0.36156) | -1 | -1 |
| G: -6290.45426 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.89111 HOMO: -5.31438 LUMO: 0.70205 factor:1 | 1 (-0.07116) | -1 | -1 |
| G: -6290.45426 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.63368 HOMO: -5.17561 LUMO: 1.04492 factor:1 | 1 (-0.81373) | -1 | -1 |
| G: -6290.45426 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.82449 HOMO: -4.94431 LUMO: 1.52656 factor:1 | 1 (-1.00454) | -1 | -1 |
| G: -6290.45426 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.62680 HOMO: -5.13751 LUMO: 0.93879 factor:1 | 1 (-0.80684) | -1 | -1 |
| G: -6290.45426 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.85341 HOMO: -5.49942 LUMO: 0.97689 factor:1 | 1 (-1.03346) | -1 | -1 |
| G: -6290.45426 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12556.43340 HOMO: -5.79058 LUMO: 0.53879 factor:1 | 1 (-1.61344) | -1 | -1 |
| G: -6290.45426 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.65975 HOMO: -5.36881 LUMO: 1.56465 factor:1 | 1 (-0.83980) | -1 | -1 |
| G: -6290.45426 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12556.13021 HOMO: -4.67492 LUMO: 1.32792 factor:1 | 1 (-1.31026) | -1 | -1 |
| G: -6290.45426 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12556.21704 HOMO: -4.60145 LUMO: 1.19458 factor:1 | 1 (-1.39709) | -1 | -1 |
| G: -6290.45426 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.49700 HOMO: -4.49260 LUMO: 1.60547 factor:1 | 1 (-0.67705) | -1 | -1 |
| G: -6290.45426 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12556.06212 HOMO: -4.65043 LUMO: 1.34696 factor:1 | 1 (-1.24217) | -1 | -1 |
| G: -6290.45426 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.34369 HOMO: -4.77560 LUMO: 1.35241 factor:1 | 1 (-0.52374) | -1 | -1 |
| G: -6290.45426 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.41808 HOMO: -4.94431 LUMO: 1.17825 factor:1 | 1 (-0.59813) | -1 | -1 |
| G: -6290.45426 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.62152 HOMO: -4.87084 LUMO: 1.41771 factor:1 | 1 (-0.80157) | -1 | -1 |
| G: -6290.45426 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.46562 HOMO: -5.34432 LUMO: 1.16737 factor:1 | 1 (-0.64567) | -1 | -1 |
| G: -6290.45426 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.23713 HOMO: -4.94975 LUMO: 1.67622 factor:1 | 1 (-0.41718) | -1 | -1 |
| G: -6290.45426 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.25264 HOMO: -4.81369 LUMO: 1.14288 factor:1 | 1 (-0.43269) | -1 | -1 |
| G: -6290.45426 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.60455 HOMO: -5.22459 LUMO: 0.29660 factor:1 | -1 (0.21541) | -1 | -1 |
| G: -6290.45426 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.38381 HOMO: -5.21642 LUMO: 0.37824 factor:1 | -1 (0.43614) | -1 | -1 |
| G: -6290.45426 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.30209 HOMO: -5.00417 LUMO: 1.01226 factor:1 | -1 (0.51786) | -1 | -1 |
| G: -6290.45426 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.56188 HOMO: -5.46677 LUMO: 0.10612 factor:1 | -1 (0.25807) | -1 | -1 |
| G: -6290.45426 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.51208 HOMO: -5.51303 LUMO: 0.54151 factor:1 | -1 (0.30787) | -1 | -1 |
| G: -6290.45426 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.11390 HOMO: -5.63004 LUMO: 0.17960 factor:1 | -1 (0.70605) | -1 | -1 |
| G: -6290.45426 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.38879 HOMO: -4.79193 LUMO: 1.12111 factor:1 | -1 (0.43116) | -1 | -1 |
| G: -6290.45426 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.31853 HOMO: -5.43411 LUMO: 0.45987 factor:1 | -1 (0.50142) | -1 | -1 |
| G: -6290.45426 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.34990 HOMO: -7.06135 LUMO: -2.13881 factor:1 | -1 (0.47005) | 1 | 1 |
| G: -6290.45426 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.18759 HOMO: -5.33071 LUMO: 1.14016 factor:1 | -1 (0.63237) | -1 | -1 |
| G: -6290.45426 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.54659 HOMO: -7.12394 LUMO: -0.03810 factor:1 | -1 (0.27337) | 1 | 1 |
| G: -6290.45426 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.32462 HOMO: -7.20558 LUMO: -2.50889 factor:1 | -1 (0.49533) | 1 | 1 |
| G: -6290.45426 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.71787 HOMO: -7.26816 LUMO: -2.11432 factor:1 | 1 (-0.89792) | 1 | 1 |
| G: -6290.45426 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12556.50834 HOMO: -7.89674 LUMO: 0.31021 factor:1 | 1 (-1.68838) | 1 | 1 |
| G: -6290.45426 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12556.25900 HOMO: -7.26544 LUMO: 0.22858 factor:1 | 1 (-1.43905) | 1 | 1 |
| G: -6290.45426 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.60573 HOMO: -7.12666 LUMO: -0.02449 factor:1 | 1 (-0.78578) | 1 | 1 |
| G: -6290.45426 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.16707 HOMO: -7.68722 LUMO: 0.71838 factor:1 | -1 (0.65288) | 1 | 1 |
| G: -6290.45426 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.39722 HOMO: -6.86271 LUMO: -0.96056 factor:1 | -1 (0.42273) | -1 | -1 |
| G: -6290.45426 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.86778 HOMO: -7.07496 LUMO: -1.11839 factor:1 | 1 (-1.04783) | 1 | 1 |
| G: -6290.45426 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.19786 HOMO: -7.06952 LUMO: -2.08439 factor:1 | 1 (-0.37791) | 1 | 1 |
| G: -6290.45426 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12556.00384 HOMO: -6.60965 LUMO: -2.11977 factor:1 | 1 (-1.18389) | -1 | -1 |
| G: -6290.45426 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.90718 HOMO: -6.87360 LUMO: -1.85854 factor:1 | 1 (-1.08723) | -1 | -1 |
| G: -6290.45426 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.69028 HOMO: -7.67089 LUMO: -0.24762 factor:1 | 1 (-0.87033) | 1 | 1 |
| G: -6290.45426 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.97155 HOMO: -6.45726 LUMO: -1.86398 factor:1 | 1 (-0.15159) | -1 | -1 |
| G: -6290.45426 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.27920 HOMO: -6.91713 LUMO: 0.33198 factor:1 | 1 (-0.45925) | -1 | -1 |
| G: -6290.45426 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.40753 HOMO: -6.83278 LUMO: 0.26667 factor:1 | 1 (-0.58758) | -1 | -1 |
| G: -6290.45426 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.37204 HOMO: -6.89264 LUMO: -1.00682 factor:1 | 1 (-0.55209) | -1 | -1 |
| G: -6290.45426 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.35400 HOMO: -6.57427 LUMO: 0.22041 factor:1 | 1 (-0.53405) | -1 | -1 |
| G: -6290.45426 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.26965 HOMO: -7.52123 LUMO: -0.01905 factor:1 | 1 (-0.44970) | 1 | 1 |
| G: -6290.45426 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.56494 HOMO: -7.37429 LUMO: -0.08980 factor:1 | 1 (-0.74499) | 1 | 1 |
| G: -6290.45426 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.58816 HOMO: -7.28449 LUMO: -0.26395 factor:1 | 1 (-0.76820) | 1 | 1 |
| G: -6290.45426 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.36513 HOMO: -6.79740 LUMO: -0.60954 factor:1 | 1 (-0.54518) | -1 | -1 |
| G: -6290.45426 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.40862 HOMO: -7.12666 LUMO: -0.60681 factor:1 | 1 (-0.58866) | 1 | 1 |
| G: -6290.45426 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.10551 HOMO: -6.96611 LUMO: -0.30477 factor:1 | 1 (-0.28556) | -1 | -1 |
| G: -6290.45426 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.22761 HOMO: -7.08040 LUMO: -0.31293 factor:1 | -1 (0.59234) | 1 | 1 |
| G: -6290.45426 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.08201 HOMO: -6.78924 LUMO: -0.73743 factor:1 | -1 (0.73795) | -1 | -1 |
| G: -6290.45426 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.09991 HOMO: -7.57293 LUMO: -1.11295 factor:1 | -1 (0.72004) | 1 | 1 |
| G: -6290.45426 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12553.83993 HOMO: -7.15932 LUMO: -0.23130 factor:1 | -1 (0.98002) | 1 | 1 |
| G: -6290.45426 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.28459 HOMO: -7.48585 LUMO: -0.10068 factor:1 | -1 (0.53536) | 1 | 1 |
| G: -6290.45426 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.99962 HOMO: -7.17020 LUMO: -0.26123 factor:1 | 1 (-1.17967) | 1 | 1 |
| G: -6290.45426 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.73978 HOMO: -7.43143 LUMO: -0.16055 factor:1 | 1 (-0.91983) | 1 | 1 |
| G: -6290.45426 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12556.05709 HOMO: -7.14843 LUMO: -0.10612 factor:1 | 1 (-1.23714) | 1 | 1 |
| G: -6290.45426 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.32848 HOMO: -6.95523 LUMO: -0.22585 factor:1 | 1 (-0.50853) | -1 | -1 |
| G: -6290.45426 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.05522 HOMO: -7.06680 LUMO: -0.51974 factor:1 | 1 (-0.23527) | 1 | 1 |
| G: -6290.45426 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.89976 HOMO: -6.80829 LUMO: -0.64763 factor:1 | 1 (-0.07981) | -1 | -1 |
| G: -6290.45426 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.09280 HOMO: -7.13210 LUMO: -0.48164 factor:1 | 1 (-0.27285) | 1 | 1 |
| G: -6290.45426 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.24516 HOMO: -7.16204 LUMO: -0.45715 factor:1 | 1 (-0.42521) | 1 | 1 |
| G: -6290.45426 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.22695 HOMO: -7.15115 LUMO: -0.43266 factor:1 | 1 (-0.40700) | 1 | 1 |
| G: -6290.45426 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.92885 HOMO: -7.15932 LUMO: -2.52794 factor:1 | 1 (-0.10890) | -1 | -1 |
| G: -6290.45426 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.04507 HOMO: -7.21102 LUMO: -2.65311 factor:1 | 1 (-0.22512) | -1 | -1 |
| G: -6290.45426 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.79405 HOMO: -6.57427 LUMO: -2.78645 factor:1 | -1 (0.02591) | -1 | -1 |
| G: -6290.45426 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.23476 HOMO: -6.40828 LUMO: -3.23815 factor:1 | 1 (-0.41481) | -1 | -1 |
| G: -6290.45426 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.38944 HOMO: -7.71987 LUMO: -0.20953 factor:1 | -1 (0.43051) | 1 | 1 |
| G: -6290.45426 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.58509 HOMO: -7.47769 LUMO: -0.43810 factor:1 | -1 (0.23486) | 1 | 1 |
| G: -6290.45426 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.52014 HOMO: -6.68040 LUMO: -2.22589 factor:1 | -1 (0.29982) | -1 | -1 |
| G: -6290.45426 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.48637 HOMO: -6.92802 LUMO: -1.99187 factor:1 | -1 (0.33358) | -1 | -1 |
| G: -6290.45426 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.19240 HOMO: -7.73620 LUMO: 0.01633 factor:1 | -1 (0.62755) | 1 | 1 |
| G: -6290.45426 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.33186 HOMO: -7.28721 LUMO: -0.18504 factor:1 | -1 (0.48809) | 1 | 1 |
| G: -6290.45426 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.55497 HOMO: -7.49674 LUMO: -0.19864 factor:1 | -1 (0.26498) | 1 | 1 |
| G: -6290.45426 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.78414 HOMO: -7.10489 LUMO: -2.56331 factor:1 | -1 (0.03581) | -1 | -1 |
| G: -6290.45426 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.75535 HOMO: -7.36612 LUMO: 0.16055 factor:1 | -1 (0.06460) | 1 | 1 |
| G: -6290.45426 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.48022 HOMO: -7.67633 LUMO: 0.33198 factor:1 | -1 (0.33973) | 1 | 1 |
| G: -6290.45426 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.55739 HOMO: -7.07768 LUMO: -0.27483 factor:1 | -1 (0.26256) | 1 | 1 |
| G: -6290.45426 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.23123 HOMO: -7.32531 LUMO: 0.05442 factor:1 | -1 (0.58872) | 1 | 1 |
| G: -6290.45426 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.33513 HOMO: -6.79740 LUMO: -1.21635 factor:1 | -1 (0.48483) | -1 | -1 |
| G: -6290.45426 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.20522 HOMO: -7.14027 LUMO: 0.12517 factor:1 | -1 (0.61473) | 1 | -1 |
| G: -6290.45426 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.04503 HOMO: -7.17292 LUMO: 0.16871 factor:1 | -1 (0.77493) | 1 | -1 |
| G: -6290.45426 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.33567 HOMO: -7.08312 LUMO: -1.38778 factor:1 | -1 (0.48428) | 1 | 1 |
| G: -6290.45426 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.57415 HOMO: -6.75387 LUMO: -1.88031 factor:1 | -1 (0.24580) | -1 | -1 |
| G: -6290.45426 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.62776 HOMO: -7.07768 LUMO: -1.25717 factor:1 | -1 (0.19219) | 1 | 1 |
| G: -6290.45426 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.35330 HOMO: -6.46543 LUMO: -1.14016 factor:1 | -1 (0.46665) | -1 | -1 |
| G: -6290.45426 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.57284 HOMO: -7.37973 LUMO: -0.45987 factor:1 | -1 (0.24711) | 1 | 1 |
| G: -6290.45426 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.47042 HOMO: -7.46408 LUMO: 0.03265 factor:1 | -1 (0.34953) | 1 | 1 |
| G: -6290.45426 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.67026 HOMO: -7.96477 LUMO: -0.19864 factor:1 | -1 (0.14969) | 1 | 1 |
| G: -6290.45426 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.17052 HOMO: -6.93890 LUMO: -1.11839 factor:1 | 1 (-0.35056) | -1 | -1 |
| G: -6290.45426 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.33591 HOMO: -7.06408 LUMO: -1.08846 factor:1 | 1 (-0.51596) | 1 | 1 |
| G: -6290.45426 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.04330 HOMO: -7.14027 LUMO: -0.33470 factor:1 | 1 (-0.22335) | 1 | 1 |
| G: -6290.45426 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.11054 HOMO: -7.38245 LUMO: 0.10885 factor:1 | 1 (-0.29059) | 1 | 1 |
| G: -6290.45426 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.02442 HOMO: -7.59470 LUMO: -1.21363 factor:1 | 1 (-0.20447) | 1 | 1 |
| G: -6290.45426 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.08181 HOMO: -7.23279 LUMO: -1.23812 factor:1 | 1 (-0.26186) | 1 | 1 |
| G: -6290.45426 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.56985 HOMO: -6.90897 LUMO: 0.23402 factor:1 | -1 (0.25010) | -1 | -1 |
| G: -6290.45426 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.31379 HOMO: -7.36340 LUMO: -0.17143 factor:1 | -1 (0.50616) | 1 | 1 |
| G: -6290.45426 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.13295 HOMO: -6.61781 LUMO: -0.01361 factor:1 | -1 (0.68701) | -1 | -1 |
| G: -6290.45426 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12553.95498 HOMO: -6.80013 LUMO: 0.38368 factor:1 | -1 (0.86497) | -1 | -1 |
| G: -6290.45426 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.25401 HOMO: -6.72121 LUMO: -0.95512 factor:1 | -1 (0.56594) | -1 | -1 |
| G: -6290.45426 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.38432 HOMO: -6.24773 LUMO: -0.69933 factor:1 | -1 (0.43563) | -1 | -1 |
| G: -6290.45426 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.34198 HOMO: -6.56883 LUMO: 0.14694 factor:1 | -1 (0.47797) | -1 | -1 |
| G: -6290.45426 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.29774 HOMO: -6.51441 LUMO: -1.27621 factor:1 | -1 (0.52221) | -1 | -1 |
| G: -6290.45426 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.05771 HOMO: -6.91986 LUMO: -1.16737 factor:1 | -1 (0.76225) | -1 | -1 |
| G: -6290.45426 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.25414 HOMO: -6.17971 LUMO: -0.65307 factor:1 | -1 (0.56581) | -1 | -1 |
| G: -6290.45426 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.15757 HOMO: -7.22462 LUMO: 0.04354 factor:1 | -1 (0.66238) | 1 | 1 |
| G: -6290.45426 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12553.84864 HOMO: -7.16204 LUMO: -0.23674 factor:1 | -1 (0.97131) | 1 | 1 |
| G: -6290.45426 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.50375 HOMO: -6.81645 LUMO: -0.19320 factor:1 | -1 (0.31620) | -1 | -1 |
| G: -6290.45426 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.16968 HOMO: -6.69400 LUMO: 0.04082 factor:1 | -1 (0.65027) | -1 | -1 |
| G: -6290.45426 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.49959 HOMO: -6.63141 LUMO: -0.22858 factor:1 | -1 (0.32036) | -1 | -1 |
| G: -6290.45426 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.33608 HOMO: -6.92258 LUMO: -1.11295 factor:1 | -1 (0.48387) | -1 | -1 |
| G: -6290.45426 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.13009 HOMO: -6.60148 LUMO: -1.13744 factor:1 | -1 (0.68986) | -1 | -1 |
| G: -6290.45426 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12553.82959 HOMO: -6.78108 LUMO: -0.82450 factor:1 | -1 (0.99036) | -1 | -1 |
| G: -6290.45426 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.32528 HOMO: -7.05591 LUMO: -0.97145 factor:1 | -1 (0.49468) | -1 | -1 |
| G: -6290.45426 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.51233 HOMO: -6.65318 LUMO: -1.26261 factor:1 | -1 (0.30762) | -1 | -1 |
| G: -6290.45426 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.45235 HOMO: -6.98244 LUMO: -0.98233 factor:1 | -1 (0.36760) | -1 | -1 |
| G: -6290.45426 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.26253 HOMO: -7.11850 LUMO: -0.99594 factor:1 | -1 (0.55743) | 1 | 1 |
| G: -6290.45426 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.26508 HOMO: -6.64230 LUMO: -0.93879 factor:1 | -1 (0.55487) | -1 | -1 |
| G: -6290.45426 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12553.90959 HOMO: -6.62053 LUMO: -1.22451 factor:1 | -1 (0.91036) | -1 | -1 |
| G: -6290.45426 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.08103 HOMO: -7.02598 LUMO: -0.85172 factor:1 | -1 (0.73893) | -1 | -1 |
| G: -6290.45426 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.10432 HOMO: -7.06680 LUMO: -0.89253 factor:1 | -1 (0.71563) | 1 | 1 |
| G: -6290.45426 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12553.83237 HOMO: -7.17292 LUMO: 0.00272 factor:1 | -1 (0.98758) | 1 | 1 |
| G: -6290.45426 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.36974 HOMO: -7.03142 LUMO: -0.35103 factor:1 | -1 (0.45021) | -1 | -1 |
| G: -6290.45426 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.66830 HOMO: -6.96884 LUMO: -0.09796 factor:1 | -1 (0.15165) | -1 | -1 |
| G: -6290.45426 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.43494 HOMO: -6.56339 LUMO: -0.99322 factor:1 | -1 (0.38501) | -1 | -1 |
| G: -6290.45426 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.58071 HOMO: -7.08857 LUMO: -0.17687 factor:1 | -1 (0.23924) | 1 | 1 |
| G: -6290.45426 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.66626 HOMO: -7.05863 LUMO: -0.22041 factor:1 | -1 (0.15369) | -1 | -1 |
| G: -6290.45426 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.72863 HOMO: -7.15115 LUMO: -0.17960 factor:1 | -1 (0.09132) | 1 | 1 |
| G: -6290.45426 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.43926 HOMO: -6.67495 LUMO: -0.96600 factor:1 | -1 (0.38069) | -1 | -1 |
| G: -6290.45426 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.39200 HOMO: -6.74026 LUMO: -1.79867 factor:1 | -1 (0.42795) | -1 | -1 |
| G: -6290.45426 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.64134 HOMO: -6.73482 LUMO: -1.78235 factor:1 | -1 (0.17862) | -1 | -1 |
| G: -6290.45426 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.34030 HOMO: -6.09807 LUMO: 0.16871 factor:1 | -1 (0.47966) | -1 | -1 |
| G: -6290.45426 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.58479 HOMO: -6.72393 LUMO: 0.27211 factor:1 | -1 (0.23516) | -1 | -1 |
| G: -6290.45426 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.62939 HOMO: -6.40556 LUMO: -0.04354 factor:1 | -1 (0.19056) | -1 | -1 |
| G: -6290.45426 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.41983 HOMO: -6.56883 LUMO: 0.22041 factor:1 | -1 (0.40012) | -1 | -1 |
| G: -6290.45426 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.28323 HOMO: -7.22462 LUMO: 0.15783 factor:1 | -1 (0.53672) | 1 | 1 |
| G: -6290.45426 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.36514 HOMO: -6.83550 LUMO: 0.19320 factor:1 | -1 (0.45481) | -1 | -1 |
| G: -6290.45426 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.48258 HOMO: -7.26816 LUMO: -0.07619 factor:1 | -1 (0.33737) | 1 | -1 |
| G: -6290.45426 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.52792 HOMO: -7.13483 LUMO: 0.33198 factor:1 | -1 (0.29203) | 1 | 1 |
| G: -6290.45426 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.32729 HOMO: -6.58243 LUMO: -0.26395 factor:1 | -1 (0.49266) | -1 | -1 |
| G: -6290.45426 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.14002 HOMO: -7.38517 LUMO: 0.17143 factor:1 | -1 (0.67993) | 1 | 1 |
| G: -6290.45426 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12553.86426 HOMO: -6.80013 LUMO: 0.25851 factor:1 | -1 (0.95569) | -1 | -1 |
| G: -6290.45426 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.39219 HOMO: -6.96611 LUMO: 0.11429 factor:1 | -1 (0.42776) | -1 | -1 |
| G: -6290.45426 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.37025 HOMO: -6.51713 LUMO: -1.14560 factor:1 | 1 (-0.55030) | -1 | -1 |
| G: -6290.45426 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.39411 HOMO: -7.15387 LUMO: -0.35647 factor:1 | 1 (-0.57416) | 1 | 1 |
| G: -6290.45426 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.37863 HOMO: -5.26540 LUMO: 1.26805 factor:1 | 1 (-0.55868) | -1 | -1 |
| G: -6290.45426 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.95620 HOMO: -6.76475 LUMO: -0.16327 factor:1 | 1 (-0.13625) | -1 | -1 |
| G: -6290.45426 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.18173 HOMO: -6.55250 LUMO: -0.71838 factor:1 | 1 (-0.36178) | -1 | -1 |
| G: -6290.45426 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.09231 HOMO: -6.76203 LUMO: -1.08301 factor:1 | 1 (-0.27236) | -1 | -1 |
| G: -6290.45426 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.16377 HOMO: -7.14027 LUMO: -0.01633 factor:1 | 1 (-0.34382) | 1 | 1 |
| G: -6290.45426 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.60196 HOMO: -6.94979 LUMO: -0.93879 factor:1 | -1 (0.21799) | -1 | -1 |
| G: -6290.45426 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.35189 HOMO: -6.74842 LUMO: 0.31293 factor:1 | -1 (0.46806) | -1 | -1 |
| G: -6290.45426 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.38612 HOMO: -6.43821 LUMO: 0.05987 factor:1 | -1 (0.43383) | -1 | -1 |
| G: -6290.45426 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.20595 HOMO: -6.60420 LUMO: 0.22585 factor:1 | -1 (0.61400) | -1 | -1 |
| G: -6290.45426 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.16097 HOMO: -6.43821 LUMO: 0.05987 factor:1 | -1 (0.65898) | -1 | -1 |
| G: -6290.45426 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.10116 HOMO: -6.34570 LUMO: 1.43948 factor:1 | -1 (0.71879) | -1 | -1 |
| G: -6290.45426 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12553.93531 HOMO: -6.03004 LUMO: 1.21363 factor:1 | -1 (0.88464) | -1 | -1 |
| G: -6290.45426 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.35110 HOMO: -6.68040 LUMO: -0.92247 factor:1 | -1 (0.46885) | -1 | -1 |
| G: -6290.45426 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.32440 HOMO: -6.92530 LUMO: -0.31293 factor:1 | -1 (0.49555) | -1 | -1 |
| G: -6290.45426 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.20744 HOMO: -6.94979 LUMO: -0.19864 factor:1 | 1 (-0.38749) | -1 | -1 |
| G: -6290.45426 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.05487 HOMO: -6.80829 LUMO: -0.30477 factor:1 | 1 (-0.23492) | -1 | -1 |
| G: -6290.45426 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.49463 HOMO: -7.22734 LUMO: -1.02859 factor:1 | 1 (-0.67468) | 1 | 1 |
| G: -6290.45426 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.84360 HOMO: -6.93890 LUMO: -0.72382 factor:1 | 1 (-0.02365) | -1 | -1 |
| G: -6290.45426 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.88308 HOMO: -7.27088 LUMO: -0.78097 factor:1 | 1 (-0.06313) | 1 | 1 |
| G: -6290.45426 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.97971 HOMO: -7.29809 LUMO: -0.97145 factor:1 | 1 (-0.15976) | 1 | 1 |
| G: -6290.45426 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.00752 HOMO: -7.18925 LUMO: -0.94696 factor:1 | 1 (-0.18757) | 1 | 1 |
| G: -6290.45426 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.14012 HOMO: -7.33891 LUMO: -0.96873 factor:1 | 1 (-0.32017) | 1 | 1 |
| G: -6290.45426 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.13383 HOMO: -7.36068 LUMO: -0.28028 factor:1 | 1 (-0.31388) | 1 | 1 |
| G: -6290.45426 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.04123 HOMO: -7.10761 LUMO: -1.14832 factor:1 | 1 (-0.22128) | 1 | 1 |
| G: -6290.45426 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.98518 HOMO: -6.94707 LUMO: -0.65307 factor:1 | 1 (-0.16523) | -1 | -1 |
| G: -6290.45426 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.75995 HOMO: -6.91713 LUMO: -1.81228 factor:1 | -1 (0.06000) | -1 | -1 |
| G: -6290.45426 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.87633 HOMO: -6.78652 LUMO: -2.01636 factor:1 | 1 (-0.05638) | -1 | -1 |
| G: -6290.45426 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.93152 HOMO: -6.52801 LUMO: -1.17553 factor:1 | 1 (-0.11157) | -1 | -1 |
| G: -6290.45426 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.22355 HOMO: -7.54844 LUMO: -1.18642 factor:1 | 1 (-0.40360) | 1 | -1 |
| G: -6290.45426 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.00306 HOMO: -7.52939 LUMO: -1.23812 factor:1 | 1 (-0.18311) | 1 | -1 |
| G: -6290.45426 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.05166 HOMO: -7.94572 LUMO: -0.81634 factor:1 | 1 (-0.23170) | 1 | 1 |
| G: -6290.45426 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.29898 HOMO: -7.55932 LUMO: -0.86260 factor:1 | 1 (-0.47903) | 1 | 1 |
| G: -6290.45426 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12556.42110 HOMO: -7.72259 LUMO: -1.39050 factor:1 | 1 (-1.60115) | 1 | -1 |
| G: -6290.45426 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.79624 HOMO: -7.11850 LUMO: -1.01498 factor:1 | 1 (-0.97629) | 1 | -1 |
| G: -6290.45426 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12556.57737 HOMO: -7.09673 LUMO: -1.00954 factor:1 | 1 (-1.75742) | 1 | -1 |
| G: -6290.45426 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.59235 HOMO: -6.06270 LUMO: 0.16327 factor:1 | 1 (-0.77240) | -1 | -1 |
| G: -6290.45426 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.61006 HOMO: -5.71167 LUMO: 0.70477 factor:1 | 1 (-0.79011) | -1 | -1 |
| G: -6290.45426 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12556.43644 HOMO: -5.38241 LUMO: 0.86260 factor:1 | 1 (-1.61649) | -1 | -1 |
| G: -6290.45426 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12556.39827 HOMO: -5.67357 LUMO: 1.27621 factor:1 | 1 (-1.57831) | -1 | -1 |
| G: -6290.45426 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12556.01633 HOMO: -7.56204 LUMO: -0.68573 factor:1 | 1 (-1.19638) | 1 | 1 |
| G: -6290.45426 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12556.39759 HOMO: -5.57833 LUMO: 1.13199 factor:1 | 1 (-1.57763) | -1 | -1 |
| G: -6290.45426 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12556.20077 HOMO: -7.58653 LUMO: -0.66124 factor:1 | 1 (-1.38081) | 1 | 1 |
| G: -6290.45426 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.41242 HOMO: -7.91851 LUMO: -1.10206 factor:1 | 1 (-0.59247) | 1 | -1 |
| G: -6290.45426 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.98346 HOMO: -6.48992 LUMO: -1.00138 factor:1 | 1 (-0.16351) | -1 | -1 |
| G: -6290.45426 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12556.16076 HOMO: -7.09673 LUMO: -0.45171 factor:1 | 1 (-1.34081) | 1 | 1 |
| G: -6290.45426 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.26867 HOMO: -6.63686 LUMO: 0.09252 factor:1 | 1 (-0.44872) | -1 | -1 |
| G: -6290.45426 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.42004 HOMO: -6.84366 LUMO: -0.14422 factor:1 | 1 (-0.60009) | -1 | -1 |
| G: -6290.45426 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.04847 HOMO: -6.93074 LUMO: 0.04354 factor:1 | 1 (-0.22852) | -1 | -1 |
| G: -6290.45426 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.61213 HOMO: -6.90353 LUMO: -0.19864 factor:1 | 1 (-0.79218) | -1 | -1 |
| G: -6290.45426 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.33278 HOMO: -6.59876 LUMO: -0.10068 factor:1 | 1 (-0.51283) | -1 | -1 |
| G: -6290.45426 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.43545 HOMO: -6.74570 LUMO: -0.44627 factor:1 | 1 (-0.61549) | -1 | -1 |
| G: -6290.45426 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.48143 HOMO: -6.60148 LUMO: -0.61770 factor:1 | 1 (-0.66148) | -1 | -1 |
| G: -6290.45426 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.35574 HOMO: -6.55794 LUMO: -1.06941 factor:1 | 1 (-0.53579) | -1 | -1 |
| G: -6290.45426 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.79926 HOMO: -7.12666 LUMO: -0.11973 factor:1 | 1 (-0.97931) | 1 | 1 |
| G: -6290.45426 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.60688 HOMO: -7.21646 LUMO: -0.50069 factor:1 | 1 (-0.78693) | 1 | 1 |
| G: -6290.45426 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.64473 HOMO: -7.27632 LUMO: -1.00682 factor:1 | 1 (-0.82478) | 1 | -1 |
| G: -6290.45426 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.61575 HOMO: -6.74298 LUMO: 0.04354 factor:1 | 1 (-0.79580) | -1 | -1 |
| G: -6290.45426 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.23956 HOMO: -6.37291 LUMO: 0.14150 factor:1 | -1 (0.58039) | -1 | -1 |
| G: -6290.45426 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.40013 HOMO: -5.61371 LUMO: 1.28438 factor:1 | -1 (0.41982) | -1 | -1 |
| G: -6290.45426 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.24974 HOMO: -5.52119 LUMO: 0.99866 factor:1 | -1 (0.57021) | -1 | -1 |
| G: -6290.45426 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.44525 HOMO: -6.51985 LUMO: -0.10885 factor:1 | -1 (0.37470) | -1 | -1 |
| G: -6290.45426 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.32143 HOMO: -5.61371 LUMO: 0.77280 factor:1 | 1 (-0.50148) | -1 | -1 |
| G: -6290.45426 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12556.03823 HOMO: -5.58922 LUMO: 0.24490 factor:1 | 1 (-1.21828) | -1 | -1 |
| G: -6290.45426 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.97173 HOMO: -6.32665 LUMO: -0.57144 factor:1 | 1 (-1.15178) | -1 | -1 |
| G: -6290.45426 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.33612 HOMO: -6.29127 LUMO: -0.93607 factor:1 | 1 (-0.51617) | -1 | -1 |
| G: -6290.45426 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.81398 HOMO: -5.49670 LUMO: 0.27211 factor:1 | 1 (-0.99403) | -1 | -1 |
| G: -6290.45426 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.16886 HOMO: -5.68990 LUMO: 0.24218 factor:1 | 1 (-0.34890) | -1 | -1 |
| G: -6290.45426 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.36393 HOMO: -5.68174 LUMO: 0.69933 factor:1 | 1 (-0.54398) | -1 | -1 |
| G: -6290.45426 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.28576 HOMO: -5.28173 LUMO: 1.00954 factor:1 | 1 (-0.46580) | -1 | -1 |
| G: -6290.45426 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.25599 HOMO: -5.94025 LUMO: 0.73471 factor:1 | 1 (-0.43604) | -1 | -1 |
| G: -6290.45426 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.29974 HOMO: -5.65725 LUMO: 1.28710 factor:1 | 1 (-0.47979) | -1 | -1 |
| G: -6290.45426 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.93582 HOMO: -5.41507 LUMO: 0.87076 factor:1 | 1 (-0.11587) | -1 | -1 |
| G: -6290.45426 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.07421 HOMO: -5.96474 LUMO: 0.29660 factor:1 | 1 (-0.25426) | -1 | -1 |
| G: -6290.45426 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.04017 HOMO: -7.00421 LUMO: 0.08708 factor:1 | 1 (-0.22022) | -1 | -1 |
| G: -6290.45426 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.86632 HOMO: -5.40418 LUMO: 0.90070 factor:1 | 1 (-0.04637) | -1 | -1 |
| G: -6290.45426 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.26083 HOMO: -7.00421 LUMO: -0.30477 factor:1 | 1 (-0.44088) | -1 | -1 |
| G: -6290.45426 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.38555 HOMO: -5.85861 LUMO: 0.74015 factor:1 | -1 (0.43440) | -1 | -1 |
| G: -6290.45426 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.45328 HOMO: -5.71439 LUMO: 0.26395 factor:1 | -1 (0.36667) | -1 | -1 |
| G: -6290.45426 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.25058 HOMO: -7.13755 LUMO: -0.78369 factor:1 | -1 (0.56937) | 1 | -1 |
| G: -6290.45426 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.45698 HOMO: -7.31442 LUMO: -0.98233 factor:1 | -1 (0.36297) | 1 | -1 |
| G: -6290.45426 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.30566 HOMO: -7.25728 LUMO: -1.00410 factor:1 | -1 (0.51430) | 1 | -1 |
| G: -6290.45426 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.44824 HOMO: -7.48585 LUMO: -0.83811 factor:1 | -1 (0.37171) | 1 | -1 |
| G: -6290.45426 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.22242 HOMO: -7.24911 LUMO: -0.77280 factor:1 | -1 (0.59753) | 1 | -1 |
| G: -6290.45426 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.42819 HOMO: -7.55116 LUMO: -1.19730 factor:1 | -1 (0.39176) | 1 | -1 |
| G: -6290.45426 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.32177 HOMO: -5.76881 LUMO: 0.28028 factor:1 | -1 (0.49819) | -1 | -1 |
| G: -6290.45426 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.26503 HOMO: -5.77153 LUMO: -0.26939 factor:1 | -1 (0.55492) | -1 | -1 |
| G: -6290.45426 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.46318 HOMO: -5.82868 LUMO: 0.36735 factor:1 | -1 (0.35677) | -1 | -1 |
| G: -6290.45426 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.29115 HOMO: -5.83140 LUMO: -0.17960 factor:1 | -1 (0.52880) | -1 | -1 |
| G: -6290.45426 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.26315 HOMO: -6.28855 LUMO: 0.01088 factor:1 | -1 (0.55680) | -1 | -1 |
| G: -6290.45426 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.31172 HOMO: -6.31576 LUMO: 0.25307 factor:1 | -1 (0.50823) | -1 | -1 |
| G: -6290.45426 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.23423 HOMO: -7.06408 LUMO: -2.76196 factor:1 | -1 (0.58573) | -1 | -1 |
| G: -6290.45426 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.36865 HOMO: -5.95657 LUMO: 0.37552 factor:1 | -1 (0.45130) | -1 | -1 |
| G: -6290.45426 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.31276 HOMO: -6.61781 LUMO: 0.02721 factor:1 | -1 (0.50719) | -1 | -1 |
| G: -6290.45426 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.51565 HOMO: -6.26678 LUMO: -0.66668 factor:1 | -1 (0.30430) | -1 | -1 |
| G: -6290.45426 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.41026 HOMO: -6.00011 LUMO: -0.13334 factor:1 | -1 (0.40969) | -1 | -1 |
| G: -6290.45426 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.28922 HOMO: -5.60555 LUMO: 0.67484 factor:1 | -1 (0.53073) | -1 | -1 |
| G: -6290.45426 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12553.97528 HOMO: -5.79875 LUMO: 0.99049 factor:1 | -1 (0.84467) | -1 | -1 |
| G: -6290.45426 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.20859 HOMO: -5.97834 LUMO: 0.48436 factor:1 | -1 (0.61136) | -1 | -1 |
| G: -6290.45426 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.40326 HOMO: -5.82868 LUMO: 0.91974 factor:1 | -1 (0.41669) | -1 | -1 |
| G: -6290.45426 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.19643 HOMO: -5.86677 LUMO: 0.99594 factor:1 | -1 (0.62352) | -1 | -1 |
| G: -6290.45426 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.41047 HOMO: -5.70079 LUMO: 0.48980 factor:1 | -1 (0.40948) | -1 | -1 |
| G: -6290.45426 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.32620 HOMO: -7.39605 LUMO: -1.02315 factor:1 | -1 (0.49375) | 1 | -1 |
| G: -6290.45426 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.23409 HOMO: -7.22734 LUMO: -1.12927 factor:1 | -1 (0.58586) | 1 | -1 |
| G: -6290.45426 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.43760 HOMO: -7.58926 LUMO: -0.65035 factor:1 | -1 (0.38235) | 1 | 1 |
| G: -6290.45426 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.50642 HOMO: -7.43959 LUMO: -0.75648 factor:1 | -1 (0.31353) | 1 | 1 |
| G: -6290.45426 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.96665 HOMO: -7.55388 LUMO: -1.15104 factor:1 | 1 (-0.14670) | 1 | -1 |
| G: -6290.45426 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.04978 HOMO: -6.74570 LUMO: -2.85447 factor:1 | 1 (-0.22983) | -1 | -1 |
| G: -6290.45426 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.90112 HOMO: -7.35524 LUMO: -1.25444 factor:1 | 1 (-0.08117) | 1 | 1 |
| G: -6290.45426 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.00159 HOMO: -6.81645 LUMO: -1.20819 factor:1 | 1 (-0.18164) | -1 | -1 |
| G: -6290.45426 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.08730 HOMO: -6.99605 LUMO: -1.62996 factor:1 | 1 (-0.26735) | -1 | -1 |
| G: -6290.45426 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.22344 HOMO: -6.88992 LUMO: -0.47620 factor:1 | 1 (-0.40349) | -1 | -1 |
| G: -6290.45426 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.36336 HOMO: -7.22190 LUMO: -0.01905 factor:1 | 1 (-0.54341) | 1 | 1 |
| G: -6290.45426 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.96719 HOMO: -6.77836 LUMO: -0.82995 factor:1 | 1 (-0.14724) | -1 | -1 |
| G: -6290.45426 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.45822 HOMO: -6.48447 LUMO: -0.95512 factor:1 | 1 (-0.63827) | -1 | -1 |
| G: -6290.45426 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12556.38678 HOMO: -7.81239 LUMO: 1.22179 factor:1 | 1 (-1.56683) | 1 | 1 |
| G: -6290.45426 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12556.16795 HOMO: -7.36612 LUMO: 0.19320 factor:1 | 1 (-1.34800) | 1 | 1 |
| G: -6290.45426 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12556.42335 HOMO: -7.24095 LUMO: 0.33470 factor:1 | 1 (-1.60340) | 1 | 1 |
| G: -6290.45426 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.50184 HOMO: -7.15932 LUMO: -2.24222 factor:1 | 1 (-0.68189) | -1 | -1 |
| G: -6290.45426 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12556.01902 HOMO: -6.88992 LUMO: -2.69937 factor:1 | 1 (-1.19907) | -1 | -1 |
| G: -6290.45426 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.41030 HOMO: -6.97428 LUMO: -0.98233 factor:1 | 1 (-0.59035) | -1 | -1 |
| G: -6290.45426 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12556.20528 HOMO: -7.17564 LUMO: -0.93879 factor:1 | 1 (-1.38533) | 1 | 1 |
| G: -6290.45426 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12556.26485 HOMO: -6.81645 LUMO: -1.14288 factor:1 | 1 (-1.44490) | -1 | -1 |
| G: -6290.45426 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.24129 HOMO: -6.83006 LUMO: -0.63403 factor:1 | 1 (-0.42134) | -1 | -1 |
| G: -6290.45426 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12556.05448 HOMO: -7.17292 LUMO: -1.07213 factor:1 | 1 (-1.23453) | 1 | 1 |
| G: -6290.45426 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.45700 HOMO: -7.53755 LUMO: 0.15510 factor:1 | 1 (-0.63705) | 1 | 1 |
| G: -6290.45426 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.27988 HOMO: -6.50080 LUMO: -0.51702 factor:1 | 1 (-0.45993) | -1 | -1 |
| G: -6290.45426 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.18823 HOMO: -6.72665 LUMO: -0.80001 factor:1 | 1 (-0.36828) | -1 | -1 |
| G: -6290.45426 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.34099 HOMO: -6.72665 LUMO: 1.68711 factor:1 | 1 (-0.52104) | -1 | -1 |
| G: -6290.45426 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.40932 HOMO: -7.11850 LUMO: -0.75103 factor:1 | 1 (-0.58937) | 1 | 1 |
| G: -6290.45426 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.26045 HOMO: -6.87087 LUMO: -0.85988 factor:1 | 1 (-0.44050) | -1 | -1 |
| G: -6290.45426 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.96940 HOMO: -7.08857 LUMO: -0.89798 factor:1 | 1 (-0.14944) | 1 | 1 |
| G: -6290.45426 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.46758 HOMO: -6.71305 LUMO: -0.85444 factor:1 | 1 (-0.64763) | -1 | -1 |
| G: -6290.45426 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.38114 HOMO: -6.59332 LUMO: -0.60137 factor:1 | -1 (0.43881) | -1 | -1 |
| G: -6290.45426 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.39728 HOMO: -7.28993 LUMO: 0.03265 factor:1 | -1 (0.42267) | 1 | 1 |
| G: -6290.45426 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.35328 HOMO: -7.32258 LUMO: 0.13878 factor:1 | -1 (0.46668) | 1 | 1 |
| G: -6290.45426 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12553.98236 HOMO: -7.28993 LUMO: 0.11429 factor:1 | -1 (0.83759) | 1 | 1 |
| G: -6290.45426 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.16582 HOMO: -6.86271 LUMO: -1.03947 factor:1 | -1 (0.65413) | -1 | -1 |
| G: -6290.45426 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.25055 HOMO: -6.55794 LUMO: -0.84900 factor:1 | -1 (0.56940) | -1 | -1 |
| G: -6290.45426 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12553.91675 HOMO: -7.03686 LUMO: 0.11429 factor:1 | -1 (0.90320) | -1 | -1 |
| G: -6290.45426 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.11776 HOMO: -7.06952 LUMO: -0.96056 factor:1 | -1 (0.70219) | 1 | 1 |
| G: -6290.45426 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.27458 HOMO: -6.90897 LUMO: -0.99866 factor:1 | -1 (0.54537) | -1 | -1 |
| G: -6290.45426 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.17681 HOMO: -7.00693 LUMO: -0.83539 factor:1 | -1 (0.64314) | -1 | -1 |
| G: -6290.45426 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.62326 HOMO: -6.74298 LUMO: -0.85172 factor:1 | 1 (-0.80331) | -1 | -1 |
| G: -6290.45426 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.35580 HOMO: -6.83822 LUMO: -1.07213 factor:1 | 1 (-0.53585) | -1 | -1 |
| G: -6290.45426 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12556.39514 HOMO: -7.21918 LUMO: -1.55377 factor:1 | 1 (-1.57519) | 1 | 1 |
| G: -6290.45426 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12556.30681 HOMO: -6.84094 LUMO: -1.09934 factor:1 | 1 (-1.48686) | -1 | -1 |
| G: -6290.45426 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12556.17853 HOMO: -7.09129 LUMO: -0.85988 factor:1 | 1 (-1.35858) | 1 | 1 |
| G: -6290.45426 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.19373 HOMO: -6.57971 LUMO: -2.27215 factor:1 | 1 (-0.37378) | -1 | -1 |
| G: -6290.45426 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12553.87792 HOMO: -6.81373 LUMO: -1.86942 factor:1 | -1 (0.94203) | -1 | -1 |
| G: -6290.45426 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.09156 HOMO: -6.59060 LUMO: -2.30480 factor:1 | -1 (0.72839) | -1 | -1 |
| G: -6290.45426 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.24691 HOMO: -6.72938 LUMO: -1.23540 factor:1 | -1 (0.57304) | -1 | -1 |
| G: -6290.45426 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.83445 HOMO: -6.94707 LUMO: -2.62318 factor:1 | 1 (-1.01449) | -1 | -1 |
| G: -6290.45426 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.80266 HOMO: -7.28177 LUMO: -0.09796 factor:1 | 1 (-0.98271) | 1 | 1 |
| G: -6290.45426 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.00401 HOMO: -6.80013 LUMO: -0.79729 factor:1 | 1 (-0.18406) | -1 | -1 |
| G: -6290.45426 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.69183 HOMO: -7.26544 LUMO: 0.12789 factor:1 | 1 (-0.87188) | 1 | 1 |
| G: -6290.45426 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.87652 HOMO: -6.51713 LUMO: -0.49253 factor:1 | 1 (-0.05657) | -1 | -1 |
| G: -6290.45426 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.90262 HOMO: -6.68856 LUMO: -0.77280 factor:1 | 1 (-0.08267) | -1 | -1 |
| G: -6290.45426 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.88136 HOMO: -6.41100 LUMO: -0.70750 factor:1 | 1 (-1.06141) | -1 | -1 |
| G: -6290.45426 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.09870 HOMO: -7.56204 LUMO: 0.22041 factor:1 | 1 (-0.27875) | 1 | 1 |
| G: -6290.45426 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.11990 HOMO: -6.68312 LUMO: 1.30343 factor:1 | 1 (-0.29995) | -1 | -1 |
| G: -6290.45426 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.23016 HOMO: -7.24367 LUMO: 0.17415 factor:1 | 1 (-0.41021) | 1 | 1 |
| G: -6289.08871 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.24925 HOMO: -7.52395 LUMO: 1.16737 factor:1 | 1 (-0.79484) | 1 | 1 |
| G: -6289.08871 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.74863 HOMO: -6.89264 LUMO: 0.23130 factor:1 | 1 (-1.29423) | -1 | -1 |
| G: -6289.08871 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12556.64135 HOMO: -7.21102 LUMO: 0.19048 factor:1 | 1 (-3.18694) | 1 | 1 |
| G: -6289.08871 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12556.08155 HOMO: -7.08312 LUMO: 0.25034 factor:1 | 1 (-2.62715) | 1 | 1 |
| G: -6289.08871 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.70810 HOMO: -6.49536 LUMO: -0.65852 factor:1 | 1 (-2.25370) | -1 | -1 |
| G: -6289.08871 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.66202 HOMO: -6.85455 LUMO: 0.13606 factor:1 | 1 (-1.20761) | -1 | -1 |
| G: -6289.08871 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.40056 HOMO: -7.10217 LUMO: 0.35919 factor:1 | 1 (-1.94616) | 1 | 1 |
| G: -6289.08871 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.48611 HOMO: -7.77429 LUMO: 1.19186 factor:1 | 1 (-2.03171) | 1 | 1 |
| G: -6289.08871 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12556.10906 HOMO: -6.57427 LUMO: -0.50069 factor:1 | 1 (-2.65466) | -1 | -1 |
| G: -6289.08871 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.41662 HOMO: -7.36340 LUMO: 0.10068 factor:1 | 1 (-1.96221) | 1 | 1 |
| G: -6289.08871 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.97246 HOMO: -7.28177 LUMO: 0.15238 factor:1 | 1 (-2.51806) | 1 | 1 |
| G: -6289.08871 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12556.00275 HOMO: -6.86543 LUMO: -0.84355 factor:1 | 1 (-2.54835) | -1 | -1 |
| G: -6289.08871 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.69451 HOMO: -6.55794 LUMO: 1.39594 factor:1 | 1 (-1.24010) | -1 | -1 |
| G: -6289.08871 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12556.08310 HOMO: -6.26134 LUMO: 1.53744 factor:1 | 1 (-2.62870) | -1 | -1 |
| G: -6289.08871 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.54884 HOMO: -5.97562 LUMO: 1.42316 factor:1 | 1 (-2.09443) | -1 | -1 |
| G: -6289.08871 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.59148 HOMO: -6.65046 LUMO: 1.44492 factor:1 | 1 (-2.13707) | -1 | -1 |
| G: -6289.08871 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.59877 HOMO: -6.92258 LUMO: 0.17415 factor:1 | 1 (-2.14437) | -1 | -1 |
| G: -6289.08871 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.65365 HOMO: -7.40966 LUMO: 0.19592 factor:1 | 1 (-2.19925) | 1 | 1 |
| G: -6289.08871 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.71919 HOMO: -7.17564 LUMO: 0.16871 factor:1 | 1 (-1.26479) | 1 | 1 |
| G: -6289.08871 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.70757 HOMO: -7.46953 LUMO: 0.22313 factor:1 | 1 (-1.25317) | 1 | 1 |
| G: -6289.08871 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.61769 HOMO: -6.13345 LUMO: 1.85854 factor:1 | 1 (-1.16329) | -1 | -1 |
| G: -6289.08871 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.72281 HOMO: -6.99333 LUMO: -1.65717 factor:1 | 1 (-1.26840) | -1 | -1 |
| G: -6289.08871 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.70787 HOMO: -6.93074 LUMO: -1.79323 factor:1 | 1 (-1.25347) | -1 | -1 |
| G: -6289.08871 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.46174 HOMO: -6.87904 LUMO: -1.79323 factor:1 | 1 (-1.00734) | -1 | -1 |
| G: -6289.08871 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12556.68480 HOMO: -6.84094 LUMO: 0.66940 factor:1 | 1 (-3.23040) | -1 | -1 |
| G: -6289.08871 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.88345 HOMO: -7.13210 LUMO: -1.17553 factor:1 | 1 (-2.42905) | 1 | 1 |
| G: -6289.08871 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.54762 HOMO: -6.52801 LUMO: -2.23678 factor:1 | 1 (-1.09322) | -1 | -1 |
| G: -6289.08871 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.96054 HOMO: -6.81917 LUMO: -1.86398 factor:1 | 1 (-2.50614) | -1 | -1 |
| G: -6289.08871 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12556.01973 HOMO: -7.30626 LUMO: -1.66806 factor:1 | 1 (-2.56533) | 1 | 1 |
| G: -6289.08871 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.38168 HOMO: -6.98516 LUMO: -1.40683 factor:1 | 1 (-1.92727) | -1 | -1 |
| G: -6289.08871 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.54633 HOMO: -6.95523 LUMO: -0.97145 factor:1 | 1 (-2.09193) | -1 | -1 |
| G: -6289.08871 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.49572 HOMO: -6.83278 LUMO: -2.68848 factor:1 | 1 (-2.04132) | -1 | -1 |
| G: -6289.08871 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.54122 HOMO: -7.25456 LUMO: -2.97420 factor:1 | 1 (-1.08682) | -1 | -1 |
| G: -6289.08871 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.57461 HOMO: -6.80557 LUMO: -2.65039 factor:1 | 1 (-1.12021) | -1 | -1 |
| G: -6289.08871 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.67320 HOMO: -7.10489 LUMO: 0.77008 factor:1 | 1 (-1.21880) | 1 | -1 |
| G: -6289.08871 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.86651 HOMO: -7.28993 LUMO: -1.06124 factor:1 | 1 (-1.41211) | 1 | 1 |
| G: -6289.08871 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.87571 HOMO: -7.11578 LUMO: -1.10206 factor:1 | 1 (-1.42131) | 1 | 1 |
| G: -6289.08871 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.81622 HOMO: -6.91713 LUMO: -1.36329 factor:1 | 1 (-1.36182) | -1 | -1 |
| G: -6289.08871 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.97568 HOMO: -7.07224 LUMO: 0.51974 factor:1 | 1 (-1.52128) | 1 | 1 |
| G: -6289.08871 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.78226 HOMO: -7.22734 LUMO: -0.93335 factor:1 | 1 (-1.32786) | 1 | 1 |
| G: -6289.08871 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.38744 HOMO: -7.19469 LUMO: -0.96600 factor:1 | 1 (-1.93304) | 1 | 1 |
| G: -6289.08871 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.52130 HOMO: -6.93890 LUMO: -0.66940 factor:1 | 1 (-2.06690) | -1 | -1 |
| G: -6289.08871 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.29925 HOMO: -7.09673 LUMO: -1.05852 factor:1 | 1 (-1.84485) | 1 | 1 |
| G: -6289.08871 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.67130 HOMO: -7.19197 LUMO: -2.26943 factor:1 | 1 (-1.21689) | -1 | -1 |
| G: -6289.08871 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.65012 HOMO: -6.90081 LUMO: -2.64767 factor:1 | 1 (-1.19572) | -1 | -1 |
| G: -6289.08871 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.82164 HOMO: -6.93890 LUMO: -2.65039 factor:1 | 1 (-1.36724) | -1 | -1 |
| G: -6289.08871 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.69924 HOMO: -6.80013 LUMO: -2.54154 factor:1 | 1 (-1.24484) | -1 | -1 |
| G: -6289.08871 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.75658 HOMO: -6.68040 LUMO: -0.89798 factor:1 | 1 (-1.30217) | -1 | -1 |
| G: -6289.08871 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.69048 HOMO: -7.01782 LUMO: -1.09662 factor:1 | 1 (-1.23608) | -1 | -1 |
| G: -6289.08871 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.39765 HOMO: -6.58516 LUMO: -0.83539 factor:1 | 1 (-1.94325) | -1 | -1 |
| G: -6289.08871 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.60682 HOMO: -7.46953 LUMO: 0.06259 factor:1 | 1 (-2.15242) | 1 | 1 |
| G: -6289.08871 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.54734 HOMO: -6.96884 LUMO: -0.99866 factor:1 | 1 (-2.09294) | -1 | -1 |
| G: -6289.08871 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.77078 HOMO: -7.29809 LUMO: -0.19320 factor:1 | 1 (-1.31638) | 1 | 1 |
| G: -6289.08871 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.25792 HOMO: -6.86271 LUMO: 0.04082 factor:1 | 1 (-1.80352) | -1 | -1 |
| G: -6289.08871 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.38347 HOMO: -6.36746 LUMO: -1.02587 factor:1 | 1 (-1.92907) | -1 | -1 |
| G: -6289.08871 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.34524 HOMO: -7.15659 LUMO: -1.25989 factor:1 | 1 (-1.89084) | 1 | 1 |
| G: -6289.08871 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.41803 HOMO: -6.69128 LUMO: -0.59865 factor:1 | 1 (-1.96363) | -1 | -1 |
| G: -6289.08871 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.18524 HOMO: -7.09129 LUMO: -1.08573 factor:1 | 1 (-1.73083) | 1 | 1 |
| G: -6289.08871 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.19827 HOMO: -6.64502 LUMO: -0.66396 factor:1 | 1 (-1.74387) | -1 | -1 |
| G: -6289.08871 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.47436 HOMO: -6.93346 LUMO: -0.87349 factor:1 | 1 (-2.01996) | -1 | -1 |
| G: -6289.08871 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12556.70061 HOMO: -6.77019 LUMO: -0.87349 factor:1 | 1 (-3.24621) | -1 | -1 |
| G: -6289.08871 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.93363 HOMO: -6.59060 LUMO: -0.82995 factor:1 | 1 (-2.47923) | -1 | -1 |
| G: -6289.08871 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.71648 HOMO: -7.17564 LUMO: -1.08846 factor:1 | 1 (-2.26208) | 1 | 1 |
| G: -6289.08871 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12556.07206 HOMO: -7.27088 LUMO: -1.18642 factor:1 | 1 (-2.61765) | 1 | 1 |
| G: -6289.08871 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.70281 HOMO: -7.06680 LUMO: -1.13199 factor:1 | 1 (-1.24840) | 1 | 1 |
| G: -6289.08871 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12556.21807 HOMO: -7.21918 LUMO: -1.03947 factor:1 | 1 (-2.76367) | 1 | 1 |
| G: -6289.08871 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.67232 HOMO: -7.26000 LUMO: -0.11973 factor:1 | 1 (-2.21792) | 1 | 1 |
| G: -6289.08871 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.76468 HOMO: -6.77564 LUMO: 0.23402 factor:1 | 1 (-1.31028) | -1 | -1 |
| G: -6289.08871 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.61064 HOMO: -7.07224 LUMO: -0.75648 factor:1 | 1 (-1.15624) | 1 | 1 |
| G: -6289.08871 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.39020 HOMO: -7.45048 LUMO: 0.18232 factor:1 | 1 (-0.93580) | 1 | 1 |
| G: -6289.08871 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.53635 HOMO: -7.48313 LUMO: 0.15238 factor:1 | 1 (-1.08195) | 1 | 1 |
| G: -6289.08871 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.68678 HOMO: -6.60692 LUMO: -0.50885 factor:1 | 1 (-1.23238) | -1 | -1 |
| G: -6289.08871 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.26336 HOMO: -6.62869 LUMO: -0.60954 factor:1 | 1 (-1.80896) | -1 | -1 |
| G: -6289.08871 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.31811 HOMO: -7.40422 LUMO: -1.28982 factor:1 | 1 (-1.86371) | 1 | 1 |
| G: -6289.08871 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.49142 HOMO: -6.75114 LUMO: -1.23268 factor:1 | 1 (-2.03702) | -1 | -1 |
| G: -6289.08871 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.65447 HOMO: -6.84638 LUMO: -0.73199 factor:1 | 1 (-2.20007) | -1 | -1 |
| G: -6289.08871 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.40562 HOMO: -6.79196 LUMO: -1.43676 factor:1 | 1 (-1.95122) | -1 | -1 |
| G: -6289.08871 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.35355 HOMO: -7.00965 LUMO: -1.37690 factor:1 | 1 (-0.89915) | -1 | -1 |
| G: -6289.08871 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.34291 HOMO: -6.97972 LUMO: -1.58098 factor:1 | 1 (-0.88851) | -1 | -1 |
| G: -6289.08871 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12556.55971 HOMO: -6.91169 LUMO: -1.48574 factor:1 | 1 (-3.10531) | -1 | -1 |
| G: -6289.08871 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.65673 HOMO: -6.90081 LUMO: -1.30343 factor:1 | 1 (-2.20233) | -1 | -1 |
| G: -6289.08871 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.31529 HOMO: -6.78652 LUMO: -1.51840 factor:1 | 1 (-0.86089) | -1 | -1 |
| G: -6289.08871 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.92762 HOMO: -6.84638 LUMO: -1.15104 factor:1 | 1 (-2.47322) | -1 | -1 |
| G: -6289.08871 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12556.04014 HOMO: -6.61237 LUMO: -0.89798 factor:1 | 1 (-2.58573) | -1 | -1 |
| G: -6289.08871 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.26508 HOMO: -7.16204 LUMO: -1.30070 factor:1 | 1 (-1.81067) | 1 | 1 |
| G: -6289.08871 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.28399 HOMO: -7.32803 LUMO: 0.14694 factor:1 | 1 (-1.82958) | 1 | 1 |
| G: -6289.08871 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.66449 HOMO: -6.99877 LUMO: -0.87621 factor:1 | 1 (-1.21009) | -1 | -1 |
| G: -6289.08871 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.76854 HOMO: -6.99877 LUMO: -0.97145 factor:1 | 1 (-2.31414) | -1 | -1 |
| G: -6289.08871 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.67120 HOMO: -7.08040 LUMO: -1.09662 factor:1 | 1 (-2.21680) | 1 | 1 |
| G: -6289.08871 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12556.20950 HOMO: -6.90897 LUMO: -1.14016 factor:1 | 1 (-2.75510) | -1 | -1 |
| G: -6289.08871 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.89138 HOMO: -6.68312 LUMO: -0.74831 factor:1 | 1 (-1.43698) | -1 | -1 |
| G: -6289.08871 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.41596 HOMO: -6.99061 LUMO: -0.86804 factor:1 | 1 (-1.96156) | -1 | -1 |
| G: -6289.08871 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.24475 HOMO: -7.10761 LUMO: -1.18642 factor:1 | 1 (-1.79035) | 1 | 1 |
| G: -6289.08871 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.00872 HOMO: -6.79196 LUMO: -0.71294 factor:1 | 1 (-1.55431) | -1 | -1 |
| G: -6289.08871 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.95936 HOMO: -6.86271 LUMO: -0.81362 factor:1 | 1 (-1.50495) | -1 | -1 |
| G: -6289.08871 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.92877 HOMO: -7.01510 LUMO: -0.99322 factor:1 | 1 (-1.47437) | -1 | -1 |
| G: -6289.08871 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.12213 HOMO: -6.88720 LUMO: -0.87893 factor:1 | 1 (-1.66773) | -1 | -1 |
| G: -6289.08871 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.97280 HOMO: -6.88448 LUMO: 0.22041 factor:1 | 1 (-1.51840) | -1 | -1 |
| G: -6289.08871 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.79601 HOMO: -7.55932 LUMO: 1.12111 factor:1 | 1 (-1.34160) | 1 | 1 |
| G: -6289.08871 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.84499 HOMO: -6.46815 LUMO: -0.86260 factor:1 | 1 (-1.39058) | -1 | -1 |
| G: -6289.08871 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.54622 HOMO: -7.13755 LUMO: 0.23130 factor:1 | 1 (-2.09182) | 1 | 1 |
| G: -6289.08871 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.50007 HOMO: -6.78924 LUMO: 1.51023 factor:1 | 1 (-2.04567) | -1 | -1 |
| G: -6289.08871 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.36304 HOMO: -6.48992 LUMO: 1.74969 factor:1 | 1 (-1.90863) | -1 | -1 |
| G: -6289.08871 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.65281 HOMO: -6.78380 LUMO: 1.81500 factor:1 | 1 (-2.19841) | -1 | -1 |
| G: -6289.08871 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.49479 HOMO: -6.49536 LUMO: 1.70615 factor:1 | 1 (-2.04039) | -1 | -1 |
| G: -6289.08871 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.53417 HOMO: -6.38651 LUMO: 1.44492 factor:1 | 1 (-2.07977) | -1 | -1 |
| G: -6289.08871 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.63851 HOMO: -6.83822 LUMO: 1.38234 factor:1 | 1 (-1.18410) | -1 | -1 |
| G: -6289.08871 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.46551 HOMO: -6.01644 LUMO: 1.20274 factor:1 | 1 (-2.01111) | -1 | -1 |
| G: -6289.08871 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.61232 HOMO: -6.18243 LUMO: 1.77962 factor:1 | 1 (-2.15792) | -1 | -1 |
| G: -6289.08871 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.45950 HOMO: -6.81917 LUMO: -1.01771 factor:1 | 1 (-2.00510) | -1 | -1 |
| G: -6289.08871 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.42383 HOMO: -6.61237 LUMO: -0.91702 factor:1 | 1 (-1.96942) | -1 | -1 |
| G: -6289.08871 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.69110 HOMO: -6.84094 LUMO: -0.84900 factor:1 | 1 (-2.23669) | -1 | -1 |
| G: -6289.08871 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.57724 HOMO: -6.81917 LUMO: -1.01771 factor:1 | 1 (-2.12284) | -1 | -1 |
| G: -6289.08871 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.68906 HOMO: -7.86953 LUMO: 1.16737 factor:1 | 1 (-2.23465) | 1 | 1 |
| G: -6289.08871 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.50249 HOMO: -7.40694 LUMO: 0.11429 factor:1 | 1 (-2.04809) | 1 | 1 |
| G: -6289.08871 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.61806 HOMO: -6.70489 LUMO: -0.65035 factor:1 | 1 (-2.16366) | -1 | -1 |
| G: -6289.08871 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.42007 HOMO: -7.23279 LUMO: 0.33470 factor:1 | 1 (-1.96567) | 1 | 1 |
| G: -6289.08871 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.34780 HOMO: -7.17020 LUMO: 0.41361 factor:1 | 1 (-1.89340) | 1 | 1 |
| G: -6289.08871 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.72836 HOMO: -6.90353 LUMO: -0.90070 factor:1 | 1 (-1.27396) | -1 | -1 |
| G: -6289.08871 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.44113 HOMO: -7.39061 LUMO: 0.17687 factor:1 | 1 (-1.98673) | 1 | 1 |
| G: -6289.08871 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.36889 HOMO: -7.16748 LUMO: 0.42178 factor:1 | 1 (-1.91448) | 1 | 1 |
| G: -6289.08871 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.38940 HOMO: -7.36884 LUMO: -1.11295 factor:1 | 1 (-1.93500) | 1 | 1 |
| G: -6289.08871 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.48356 HOMO: -7.33347 LUMO: 0.33198 factor:1 | 1 (-2.02915) | 1 | 1 |
| G: -6289.08871 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.59907 HOMO: -7.31986 LUMO: -0.83539 factor:1 | 1 (-2.14467) | 1 | 1 |
| G: -6289.08871 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.71172 HOMO: -7.31170 LUMO: 0.08708 factor:1 | 1 (-2.25732) | 1 | 1 |
| G: -6289.08871 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.87701 HOMO: -7.36884 LUMO: 0.38096 factor:1 | 1 (-1.42261) | 1 | 1 |
| G: -6289.08871 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.32080 HOMO: -6.99333 LUMO: 1.74153 factor:1 | 1 (-1.86640) | -1 | -1 |
| G: -6289.08871 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.98714 HOMO: -6.94435 LUMO: 1.74969 factor:1 | 1 (-1.53274) | -1 | -1 |
| G: -6289.08871 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.27427 HOMO: -7.02598 LUMO: 1.43404 factor:1 | 1 (-1.81987) | -1 | -1 |
| G: -6289.08871 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.02586 HOMO: -6.41100 LUMO: 1.62996 factor:1 | 1 (-1.57146) | -1 | -1 |
| G: -6289.08871 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.39237 HOMO: -6.57699 LUMO: 1.81228 factor:1 | 1 (-1.93797) | -1 | -1 |
| G: -6289.08871 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.46897 HOMO: -6.86543 LUMO: 1.49935 factor:1 | 1 (-2.01457) | -1 | -1 |
| G: -6289.08871 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.46252 HOMO: -6.91169 LUMO: -1.22451 factor:1 | 1 (-2.00812) | -1 | -1 |
| G: -6289.08871 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.44023 HOMO: -7.09945 LUMO: -1.23812 factor:1 | 1 (-1.98583) | 1 | 1 |
| G: -6289.08871 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.04311 HOMO: -7.48857 LUMO: 0.10340 factor:1 | 1 (-1.58871) | 1 | 1 |
| G: -6289.08871 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.00779 HOMO: -7.21918 LUMO: -0.06803 factor:1 | 1 (-1.55339) | 1 | 1 |
| G: -6289.08871 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.26616 HOMO: -6.34025 LUMO: -0.68845 factor:1 | 1 (-1.81176) | -1 | -1 |
| G: -6289.08871 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.14711 HOMO: -6.82734 LUMO: -0.77825 factor:1 | 1 (-1.69271) | -1 | -1 |
| G: -6289.08871 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.10635 HOMO: -6.92258 LUMO: -1.03675 factor:1 | 1 (-1.65195) | -1 | -1 |
| G: -6289.08871 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.73323 HOMO: -6.42461 LUMO: -0.95240 factor:1 | 1 (-1.27883) | -1 | -1 |
| G: -6289.08871 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.92801 HOMO: -6.96067 LUMO: -1.05036 factor:1 | 1 (-1.47361) | -1 | -1 |
| G: -6289.08871 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.91440 HOMO: -7.23551 LUMO: 0.12245 factor:1 | 1 (-1.46000) | 1 | 1 |
| G: -6289.08871 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.85573 HOMO: -6.85183 LUMO: 0.16055 factor:1 | 1 (-1.40133) | -1 | -1 |
| G: -6289.08871 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.48422 HOMO: -6.46815 LUMO: -0.89253 factor:1 | 1 (-1.02981) | -1 | -1 |
| G: -6289.08871 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.99331 HOMO: -7.23823 LUMO: -0.06259 factor:1 | 1 (-1.53891) | 1 | 1 |
| G: -6289.08871 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.62117 HOMO: -6.76475 LUMO: -0.99049 factor:1 | 1 (-1.16677) | -1 | -1 |
| G: -6289.08871 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.35904 HOMO: -7.14843 LUMO: -0.88165 factor:1 | 1 (-1.90463) | 1 | 1 |
| G: -6289.08871 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.89507 HOMO: -7.15659 LUMO: 0.20681 factor:1 | 1 (-2.44067) | 1 | 1 |
| G: -6289.08871 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.85657 HOMO: -7.11306 LUMO: 0.14150 factor:1 | 1 (-2.40217) | 1 | 1 |
| G: -6289.08871 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12556.42352 HOMO: -6.67223 LUMO: -0.86260 factor:1 | 1 (-2.96912) | -1 | -1 |
| G: -6289.08871 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12556.25546 HOMO: -6.92530 LUMO: 0.30749 factor:1 | 1 (-2.80106) | -1 | -1 |
| G: -6289.08871 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.93594 HOMO: -6.50624 LUMO: -0.70477 factor:1 | 1 (-2.48154) | -1 | -1 |
| G: -6289.08871 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.54247 HOMO: -7.35524 LUMO: 0.75103 factor:1 | 1 (-2.08807) | 1 | 1 |
| G: -6289.08871 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.85921 HOMO: -7.07768 LUMO: -0.26939 factor:1 | 1 (-2.40481) | 1 | 1 |
| G: -6289.08871 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.81126 HOMO: -7.15932 LUMO: 0.42450 factor:1 | 1 (-2.35686) | 1 | 1 |
| G: -6289.08871 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12556.06357 HOMO: -7.46136 LUMO: 0.04626 factor:1 | 1 (-2.60916) | 1 | 1 |
| G: -6289.08871 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12556.39748 HOMO: -7.05047 LUMO: -1.06669 factor:1 | 1 (-2.94307) | -1 | -1 |
| G: -6289.08871 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12556.39677 HOMO: -6.66951 LUMO: -0.99322 factor:1 | 1 (-2.94237) | -1 | -1 |
| G: -6289.08871 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12556.55440 HOMO: -7.01782 LUMO: -1.08846 factor:1 | 1 (-3.10000) | -1 | -1 |
| G: -6289.08871 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.91496 HOMO: -7.03959 LUMO: -1.15376 factor:1 | 1 (-2.46056) | -1 | -1 |
| G: -6289.08871 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12556.60692 HOMO: -6.68856 LUMO: 1.61364 factor:1 | 1 (-3.15252) | -1 | -1 |
| G: -6289.08871 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12556.45731 HOMO: -6.53345 LUMO: 1.60275 factor:1 | 1 (-3.00291) | -1 | -1 |
| G: -6289.08871 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.65442 HOMO: -6.73482 LUMO: 1.86398 factor:1 | 1 (-2.20001) | -1 | -1 |
| G: -6289.08871 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.88794 HOMO: -6.87632 LUMO: 1.59731 factor:1 | 1 (-2.43354) | -1 | -1 |
| G: -6289.08871 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12556.57098 HOMO: -6.31848 LUMO: 2.12521 factor:1 | 1 (-3.11657) | -1 | -1 |
| G: -6289.08871 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12556.44131 HOMO: -6.35114 LUMO: 1.71432 factor:1 | 1 (-2.98691) | -1 | -1 |
| G: -6289.08871 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12556.10923 HOMO: -6.34842 LUMO: 1.92929 factor:1 | 1 (-2.65482) | -1 | -1 |
| G: -6289.08871 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.84634 HOMO: -6.14977 LUMO: 1.78235 factor:1 | 1 (-2.39194) | -1 | -1 |
| G: -6289.08871 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.55694 HOMO: -6.31032 LUMO: 1.51567 factor:1 | 1 (-2.10254) | -1 | -1 |
| G: -6289.08871 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.41551 HOMO: -6.25862 LUMO: 1.75241 factor:1 | 1 (-0.96111) | -1 | -1 |
| G: -6289.08871 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.28005 HOMO: -6.49264 LUMO: 1.66806 factor:1 | 1 (-0.82565) | -1 | -1 |
| G: -6289.08871 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.44350 HOMO: -6.28311 LUMO: 1.60003 factor:1 | 1 (-1.98910) | -1 | -1 |
| G: -6289.08871 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.49281 HOMO: -7.13210 LUMO: -0.04354 factor:1 | 1 (-2.03840) | 1 | 1 |
| G: -6289.08871 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.68609 HOMO: -7.35252 LUMO: 0.03537 factor:1 | 1 (-2.23169) | 1 | 1 |
| G: -6289.08871 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.37958 HOMO: -6.58243 LUMO: -0.48980 factor:1 | 1 (-1.92518) | -1 | -1 |
| G: -6289.08871 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.79856 HOMO: -6.90081 LUMO: -0.05442 factor:1 | 1 (-1.34416) | -1 | -1 |
| G: -6289.08871 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.65685 HOMO: -7.22734 LUMO: 0.17143 factor:1 | 1 (-1.20244) | 1 | 1 |
| G: -6289.08871 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.57687 HOMO: -7.13210 LUMO: -0.99866 factor:1 | 1 (-1.12247) | 1 | 1 |
| G: -6289.08871 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.75309 HOMO: -7.39878 LUMO: 0.13334 factor:1 | 1 (-1.29869) | 1 | 1 |
| G: -6289.08871 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.74934 HOMO: -7.04503 LUMO: -0.89798 factor:1 | 1 (-1.29494) | -1 | -1 |
| G: -6289.08871 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.45328 HOMO: -6.95523 LUMO: -1.07213 factor:1 | 1 (-0.99888) | -1 | -1 |
| G: -6289.08871 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12556.04680 HOMO: -6.75114 LUMO: -1.28438 factor:1 | 1 (-2.59240) | -1 | -1 |
| G: -6289.08871 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12556.48874 HOMO: -6.75114 LUMO: -0.11701 factor:1 | 1 (-3.03434) | -1 | -1 |
| G: -6289.08871 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.55527 HOMO: -6.83278 LUMO: -0.01633 factor:1 | 1 (-1.10086) | -1 | -1 |
| G: -6289.08871 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.89015 HOMO: -6.93890 LUMO: -0.88981 factor:1 | 1 (-2.43575) | -1 | -1 |
| G: -6289.08871 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.23318 HOMO: -7.07224 LUMO: -1.08573 factor:1 | 1 (-1.77878) | 1 | 1 |
| G: -6289.08871 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.55499 HOMO: -6.99877 LUMO: -0.95240 factor:1 | 1 (-2.10058) | -1 | -1 |
| G: -6289.08871 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12556.12569 HOMO: -7.09129 LUMO: 0.35375 factor:1 | 1 (-2.67129) | 1 | 1 |
| G: -6289.08871 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.77570 HOMO: -7.09401 LUMO: 0.04354 factor:1 | 1 (-2.32129) | 1 | 1 |
| G: -6289.08871 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.51722 HOMO: -6.85183 LUMO: -0.68573 factor:1 | 1 (-2.06281) | -1 | -1 |
| G: -6289.08871 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.43194 HOMO: -6.83006 LUMO: -0.58777 factor:1 | 1 (-1.97753) | -1 | -1 |
| G: -6289.08871 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.58217 HOMO: -7.40422 LUMO: 0.17687 factor:1 | 1 (-2.12777) | 1 | 1 |
| G: -6289.08871 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.21248 HOMO: -7.15932 LUMO: 0.10340 factor:1 | 1 (-1.75807) | 1 | 1 |
| G: -6289.08871 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.55833 HOMO: -7.03414 LUMO: -0.19592 factor:1 | 1 (-2.10393) | -1 | -1 |
| G: -6289.08871 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.85545 HOMO: -6.48447 LUMO: -0.36191 factor:1 | 1 (-2.40105) | -1 | -1 |
| G: -6289.08871 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.42883 HOMO: -7.49402 LUMO: 0.11429 factor:1 | 1 (-1.97443) | 1 | 1 |
| G: -6289.08871 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.27749 HOMO: -7.01237 LUMO: -1.06397 factor:1 | 1 (-0.82309) | -1 | -1 |
| G: -6289.08871 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.46408 HOMO: -6.67223 LUMO: -1.07213 factor:1 | 1 (-1.00968) | -1 | -1 |
| G: -6289.08871 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12553.99694 HOMO: -7.38789 LUMO: -1.15376 factor:1 | 1 (-0.54254) | 1 | 1 |
| G: -6289.08871 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.56631 HOMO: -6.42461 LUMO: -1.23812 factor:1 | 1 (-1.11191) | -1 | -1 |
| G: -6289.08871 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.33210 HOMO: -7.36884 LUMO: -1.19186 factor:1 | 1 (-1.87769) | 1 | 1 |
| G: -6289.08871 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.94101 HOMO: -6.65591 LUMO: 0.07075 factor:1 | 1 (-2.48660) | -1 | -1 |
| G: -6289.08871 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.48211 HOMO: -7.39061 LUMO: -0.16871 factor:1 | 1 (-2.02771) | 1 | 1 |
| G: -6289.08871 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.18861 HOMO: -6.90353 LUMO: -0.96056 factor:1 | 1 (-1.73421) | -1 | -1 |
| G: -6289.08871 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.86854 HOMO: -7.42054 LUMO: 0.19048 factor:1 | 1 (-2.41414) | 1 | 1 |
| G: -6289.08871 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.79665 HOMO: -7.40150 LUMO: 0.35647 factor:1 | 1 (-2.34225) | 1 | 1 |
| G: -6289.08871 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.95600 HOMO: -6.56067 LUMO: -0.96056 factor:1 | 1 (-2.50160) | -1 | -1 |
| G: -6289.08871 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.59431 HOMO: -6.89809 LUMO: -0.81090 factor:1 | 1 (-2.13990) | -1 | -1 |
| G: -6289.08871 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.42780 HOMO: -6.91986 LUMO: -0.84900 factor:1 | 1 (-1.97340) | -1 | -1 |
| G: -6289.08871 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.37030 HOMO: -6.61509 LUMO: -0.62042 factor:1 | 1 (-1.91590) | -1 | -1 |
| G: -6289.08871 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.71711 HOMO: -6.58243 LUMO: -0.65579 factor:1 | 1 (-2.26271) | -1 | -1 |
| G: -6289.08871 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.42543 HOMO: -6.52257 LUMO: -0.92519 factor:1 | 1 (-1.97103) | -1 | -1 |
| G: -6289.08871 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.78242 HOMO: -6.69128 LUMO: 1.49118 factor:1 | 1 (-2.32802) | -1 | -1 |
| G: -6289.08871 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.82971 HOMO: -7.02870 LUMO: 1.67894 factor:1 | 1 (-2.37531) | -1 | -1 |
| G: -6289.08871 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.97521 HOMO: -6.88720 LUMO: 1.68711 factor:1 | 1 (-2.52081) | -1 | -1 |
| G: -6289.08871 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.66103 HOMO: -5.89943 LUMO: 1.03675 factor:1 | 1 (-2.20663) | -1 | -1 |
| G: -6289.08871 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.51219 HOMO: -6.40556 LUMO: 1.14560 factor:1 | 1 (-1.05779) | -1 | -1 |
| G: -6289.08871 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.43222 HOMO: -6.51168 LUMO: 1.48030 factor:1 | 1 (-0.97781) | -1 | -1 |
| G: -6289.08871 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.61187 HOMO: -6.64502 LUMO: 1.91568 factor:1 | 1 (-1.15746) | -1 | -1 |
| G: -6289.08871 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.32040 HOMO: -6.47903 LUMO: 1.91296 factor:1 | 1 (-0.86600) | -1 | -1 |
| G: -6289.08871 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.59978 HOMO: -6.34297 LUMO: 1.91840 factor:1 | 1 (-1.14538) | -1 | -1 |
| G: -6289.08871 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.40179 HOMO: -6.89809 LUMO: 1.82861 factor:1 | 1 (-1.94738) | -1 | -1 |
| G: -6289.08871 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.97271 HOMO: -6.10079 LUMO: 1.62996 factor:1 | 1 (-2.51830) | -1 | -1 |
| G: -6289.08871 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.34627 HOMO: -7.16476 LUMO: -0.92247 factor:1 | 1 (-1.89187) | 1 | 1 |
| G: -6289.08871 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12556.20109 HOMO: -7.10489 LUMO: -0.95784 factor:1 | 1 (-2.74669) | 1 | 1 |
| G: -6289.08871 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.54625 HOMO: -6.76475 LUMO: -0.99866 factor:1 | 1 (-2.09185) | -1 | -1 |
| G: -6289.08871 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.88593 HOMO: -6.81373 LUMO: -1.05036 factor:1 | 1 (-2.43153) | -1 | -1 |
| G: -6289.08871 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.32987 HOMO: -6.90081 LUMO: -1.03947 factor:1 | 1 (-1.87546) | -1 | -1 |
| G: -6289.08871 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.18616 HOMO: -7.06952 LUMO: -0.91702 factor:1 | 1 (-1.73176) | 1 | 1 |
| G: -6289.08871 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.41874 HOMO: -6.73482 LUMO: -0.94151 factor:1 | 1 (-1.96434) | -1 | -1 |
| G: -6289.08871 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.47463 HOMO: -6.99605 LUMO: -1.04764 factor:1 | 1 (-2.02023) | -1 | -1 |
| G: -6289.08871 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.20216 HOMO: -7.03686 LUMO: -0.93335 factor:1 | 1 (-1.74776) | -1 | -1 |
| G: -6289.08871 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.10755 HOMO: -6.81101 LUMO: -0.95240 factor:1 | 1 (-1.65315) | -1 | -1 |
| G: -6289.08871 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.89584 HOMO: -6.83822 LUMO: -0.65307 factor:1 | 1 (-1.44144) | -1 | -1 |
| G: -6289.08871 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.05076 HOMO: -7.05319 LUMO: -0.81634 factor:1 | 1 (-1.59636) | -1 | -1 |
| G: -6289.08871 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.35009 HOMO: -7.57565 LUMO: 0.19048 factor:1 | 1 (-0.89569) | 1 | 1 |
| G: -6289.08871 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.53429 HOMO: -6.56067 LUMO: -0.50613 factor:1 | 1 (-1.07988) | -1 | -1 |
| G: -6289.08871 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.68240 HOMO: -6.74298 LUMO: -0.70477 factor:1 | 1 (-1.22800) | -1 | -1 |
| G: -6289.08871 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.84537 HOMO: -7.02054 LUMO: 0.03537 factor:1 | 1 (-1.39096) | -1 | -1 |
| G: -6289.08871 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.72025 HOMO: -7.33347 LUMO: -0.17960 factor:1 | 1 (-1.26585) | 1 | 1 |
| G: -6289.08871 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.33523 HOMO: -6.98244 LUMO: -0.88165 factor:1 | 1 (-0.88083) | -1 | -1 |
| G: -6289.08871 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.41393 HOMO: -7.14843 LUMO: -1.19730 factor:1 | 1 (-0.95953) | 1 | 1 |
| G: -6289.08871 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.74822 HOMO: -7.17564 LUMO: -1.21907 factor:1 | 1 (-1.29382) | 1 | 1 |
| G: -6289.08871 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.38854 HOMO: -6.74026 LUMO: -0.86532 factor:1 | 1 (-0.93414) | -1 | -1 |
| G: -6289.08871 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.62724 HOMO: -6.82462 LUMO: -1.24084 factor:1 | 1 (-1.17284) | -1 | -1 |
| G: -6289.08871 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.29366 HOMO: -6.78924 LUMO: -0.70477 factor:1 | 1 (-0.83925) | -1 | -1 |
| G: -6289.08871 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.77864 HOMO: -7.41238 LUMO: 0.05987 factor:1 | 1 (-1.32424) | 1 | 1 |
| G: -6289.08871 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.46397 HOMO: -6.75931 LUMO: 0.02721 factor:1 | 1 (-1.00957) | -1 | -1 |
| G: -6289.08871 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.63271 HOMO: -6.28583 LUMO: -0.93063 factor:1 | 1 (-1.17831) | -1 | -1 |
| G: -6289.08871 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.62936 HOMO: -6.69128 LUMO: -0.83539 factor:1 | 1 (-1.17496) | -1 | -1 |
| G: -6289.08871 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.30228 HOMO: -7.22190 LUMO: 0.01361 factor:1 | 1 (-0.84788) | 1 | 1 |
| G: -6289.08871 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.20144 HOMO: -6.95251 LUMO: -1.09934 factor:1 | 1 (-0.74703) | -1 | -1 |
| G: -6289.08871 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.38955 HOMO: -6.75387 LUMO: -0.90614 factor:1 | 1 (-0.93515) | -1 | -1 |
| G: -6289.08871 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.42691 HOMO: -7.48585 LUMO: 0.05987 factor:1 | 1 (-0.97251) | 1 | 1 |
| G: -6289.08871 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.53001 HOMO: -6.92802 LUMO: -0.66940 factor:1 | 1 (-1.07561) | -1 | -1 |
| G: -6289.08871 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.44019 HOMO: -7.29537 LUMO: -0.14150 factor:1 | 1 (-0.98579) | 1 | 1 |
| G: -6289.08871 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.25118 HOMO: -6.57155 LUMO: -0.86804 factor:1 | 1 (-0.79678) | -1 | -1 |
| G: -6289.08871 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.74692 HOMO: -6.87632 LUMO: -0.77825 factor:1 | 1 (-1.29251) | -1 | -1 |
| G: -6289.08871 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.66773 HOMO: -6.45998 LUMO: -0.31565 factor:1 | 1 (-1.21333) | -1 | -1 |
| G: -6289.08871 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.80055 HOMO: -7.51306 LUMO: 0.05714 factor:1 | 1 (-1.34615) | 1 | 1 |
| G: -6289.08871 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.66735 HOMO: -6.86271 LUMO: -0.00816 factor:1 | 1 (-1.21295) | -1 | -1 |
| G: -6289.08871 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.41320 HOMO: -6.43277 LUMO: -1.07485 factor:1 | 1 (-0.95879) | -1 | -1 |
| G: -6289.08871 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.52378 HOMO: -6.78108 LUMO: -0.81362 factor:1 | 1 (-1.06938) | -1 | -1 |
| G: -6289.08871 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.56373 HOMO: -6.88448 LUMO: 1.21907 factor:1 | 1 (-1.10933) | -1 | -1 |
| G: -6289.08871 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.19877 HOMO: -6.97700 LUMO: 1.44765 factor:1 | 1 (-0.74437) | -1 | -1 |
| G: -6289.08871 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.26500 HOMO: -6.89537 LUMO: 2.12249 factor:1 | 1 (-0.81060) | -1 | -1 |
| G: -6289.08871 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.42604 HOMO: -6.28311 LUMO: 1.45037 factor:1 | 1 (-0.97164) | -1 | -1 |
| G: -6289.08871 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.46571 HOMO: -6.55522 LUMO: 1.39867 factor:1 | 1 (-1.01131) | -1 | -1 |
| G: -6289.08871 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.56142 HOMO: -6.46815 LUMO: 1.50207 factor:1 | 1 (-1.10701) | -1 | -1 |
| G: -6289.08871 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.54381 HOMO: -6.43549 LUMO: 2.17419 factor:1 | 1 (-1.08941) | -1 | -1 |
| G: -6289.08871 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.67834 HOMO: -6.99333 LUMO: 1.87214 factor:1 | 1 (-1.22394) | -1 | -1 |
| G: -6289.08871 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.42332 HOMO: -6.65591 LUMO: 1.37962 factor:1 | 1 (-0.96892) | -1 | -1 |
| G: -6289.08871 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.46095 HOMO: -6.82734 LUMO: 1.55649 factor:1 | 1 (-1.00655) | -1 | -1 |
| G: -6289.08871 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.10170 HOMO: -6.71849 LUMO: 1.36057 factor:1 | 1 (-1.64730) | -1 | -1 |
| G: -6289.08871 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.20706 HOMO: -6.79468 LUMO: 1.82044 factor:1 | 1 (-1.75266) | -1 | -1 |
| G: -6289.08871 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.30053 HOMO: -6.61237 LUMO: 1.15104 factor:1 | 1 (-1.84613) | -1 | -1 |
| G: -6289.08871 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.34951 HOMO: -6.62053 LUMO: 2.33474 factor:1 | 1 (-1.89511) | -1 | -1 |
| G: -6289.08871 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.98787 HOMO: -6.55794 LUMO: 1.65717 factor:1 | 1 (-1.53347) | -1 | -1 |
| G: -6289.08871 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.99492 HOMO: -6.85999 LUMO: 2.03813 factor:1 | 1 (-1.54052) | -1 | -1 |
| G: -6289.08871 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.35988 HOMO: -6.45726 LUMO: 1.28438 factor:1 | 1 (-1.90548) | -1 | -1 |
| G: -6289.08871 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.15843 HOMO: -6.23685 LUMO: 1.93201 factor:1 | 1 (-1.70403) | -1 | -1 |
| G: -6289.08871 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.70421 HOMO: -7.06680 LUMO: 1.86942 factor:1 | 1 (-2.24981) | 1 | 1 |
| G: -6289.08871 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.80133 HOMO: -6.89537 LUMO: 2.17147 factor:1 | 1 (-2.34693) | -1 | -1 |
| G: -6289.08871 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12556.57601 HOMO: -6.80013 LUMO: 1.78779 factor:1 | 1 (-3.12161) | -1 | -1 |
| G: -6289.08871 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12556.55519 HOMO: -6.45726 LUMO: 1.58370 factor:1 | 1 (-3.10079) | -1 | -1 |
| G: -6289.08871 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.83722 HOMO: -6.52529 LUMO: 1.71976 factor:1 | 1 (-2.38282) | -1 | -1 |
| G: -6289.08871 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12556.40556 HOMO: -7.22462 LUMO: -1.18642 factor:1 | 1 (-2.95116) | 1 | 1 |
| G: -6289.08871 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12556.27206 HOMO: -7.18381 LUMO: -0.78641 factor:1 | 1 (-2.81766) | 1 | 1 |
| G: -6289.08871 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.60386 HOMO: -6.93346 LUMO: 1.65717 factor:1 | 1 (-2.14945) | -1 | -1 |
| G: -6289.08871 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12556.09045 HOMO: -6.41644 LUMO: 1.78235 factor:1 | 1 (-2.63605) | -1 | -1 |
| G: -6289.08871 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.45866 HOMO: -6.59876 LUMO: 1.83677 factor:1 | 1 (-2.00425) | -1 | -1 |
| G: -6289.08871 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.46579 HOMO: -6.35658 LUMO: 1.59731 factor:1 | 1 (-2.01138) | -1 | -1 |
| G: -6289.08871 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.36274 HOMO: -6.60692 LUMO: 1.66534 factor:1 | 1 (-1.90833) | -1 | -1 |
| G: -6289.08871 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.71178 HOMO: -6.83006 LUMO: 2.11705 factor:1 | 1 (-2.25737) | -1 | -1 |
| G: -6289.08871 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.39857 HOMO: -6.89264 LUMO: 1.30070 factor:1 | 1 (-1.94417) | -1 | -1 |
| G: -6289.08871 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.61440 HOMO: -6.90081 LUMO: 2.05174 factor:1 | 1 (-1.15999) | -1 | -1 |
| G: -6289.08871 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.61851 HOMO: -6.74842 LUMO: 1.96194 factor:1 | 1 (-1.16410) | -1 | -1 |
| G: -6289.08871 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.30334 HOMO: -6.58516 LUMO: 1.30887 factor:1 | 1 (-0.84894) | -1 | -1 |
| G: -6289.08871 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.71309 HOMO: -7.00965 LUMO: 2.08167 factor:1 | 1 (-1.25869) | -1 | -1 |
| G: -6289.08871 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.50000 HOMO: -6.86815 LUMO: 2.29664 factor:1 | 1 (-1.04560) | -1 | -1 |
| G: -6289.08871 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.29050 HOMO: -6.39740 LUMO: 2.02725 factor:1 | 1 (-0.83610) | -1 | -1 |
| G: -6289.08871 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.54531 HOMO: -5.95929 LUMO: 1.62724 factor:1 | 1 (-1.09090) | -1 | -1 |
| G: -6289.08871 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.39230 HOMO: -6.71849 LUMO: 1.34696 factor:1 | 1 (-0.93789) | -1 | -1 |
| G: -6289.08871 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.87047 HOMO: -7.26816 LUMO: 1.74153 factor:1 | 1 (-2.41607) | 1 | 1 |
| G: -6289.08871 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12556.40550 HOMO: -6.90897 LUMO: 1.71432 factor:1 | 1 (-2.95110) | -1 | -1 |
| G: -6289.08871 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.53828 HOMO: -6.70489 LUMO: 1.91568 factor:1 | 1 (-2.08388) | -1 | -1 |
| G: -6289.08871 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12556.52069 HOMO: -6.83278 LUMO: 1.61908 factor:1 | 1 (-3.06629) | -1 | -1 |
| G: -6289.08871 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12556.22874 HOMO: -7.17292 LUMO: 1.95378 factor:1 | 1 (-2.77434) | 1 | -1 |
| G: -6289.08871 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.26968 HOMO: -6.53345 LUMO: 1.74153 factor:1 | 1 (-0.81528) | -1 | -1 |
| G: -6289.08871 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.48653 HOMO: -6.53073 LUMO: 1.51023 factor:1 | 1 (-1.03213) | -1 | -1 |
| G: -6289.08871 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.27308 HOMO: -6.93346 LUMO: 2.22861 factor:1 | 1 (-0.81868) | -1 | -1 |
| G: -6289.08871 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.87967 HOMO: -6.47903 LUMO: 2.05446 factor:1 | 1 (-2.42527) | -1 | -1 |
| G: -6289.08871 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.10967 HOMO: -6.88992 LUMO: 1.57010 factor:1 | 1 (-1.65527) | -1 | -1 |
| G: -6289.08871 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.28453 HOMO: -6.07358 LUMO: 1.95922 factor:1 | 1 (-1.83013) | -1 | -1 |
| G: -6289.08871 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12556.05744 HOMO: -6.75114 LUMO: 2.18780 factor:1 | 1 (-2.60304) | -1 | -1 |
| G: -6289.08871 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.19008 HOMO: -6.96339 LUMO: 1.70071 factor:1 | 1 (-1.73568) | -1 | -1 |
| G: -6289.08871 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.80177 HOMO: -7.14843 LUMO: 1.82588 factor:1 | 1 (-2.34736) | 1 | -1 |
| G: -6289.08871 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.96692 HOMO: -6.96339 LUMO: 2.29392 factor:1 | 1 (-1.51252) | -1 | -1 |
| G: -6289.08871 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.46219 HOMO: -6.81645 LUMO: 2.39732 factor:1 | 1 (-2.00779) | -1 | -1 |
| G: -6289.08871 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.51469 HOMO: -6.48447 LUMO: 1.24084 factor:1 | 1 (-2.06028) | -1 | -1 |
| G: -6289.08871 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.28654 HOMO: -7.14843 LUMO: 2.01092 factor:1 | 1 (-1.83214) | 1 | -1 |
| G: -6289.08871 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.33955 HOMO: -7.20013 LUMO: -0.34286 factor:1 | 1 (-1.88515) | 1 | -1 |
| G: -6289.08871 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.43308 HOMO: -6.97700 LUMO: -0.15238 factor:1 | 1 (-1.97868) | -1 | -1 |
| G: -6289.08871 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.27237 HOMO: -7.07768 LUMO: -0.26123 factor:1 | 1 (-1.81797) | 1 | -1 |
| G: -6289.08871 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.29114 HOMO: -6.99333 LUMO: -0.41361 factor:1 | 1 (-1.83674) | -1 | -1 |
| G: -6289.08871 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.09334 HOMO: -6.84638 LUMO: -0.40273 factor:1 | 1 (-1.63894) | -1 | -1 |
| G: -6289.08871 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.70125 HOMO: -6.83822 LUMO: -0.26939 factor:1 | 1 (-2.24684) | -1 | -1 |
| G: -6289.08871 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.47221 HOMO: -6.75931 LUMO: -0.93879 factor:1 | 1 (-2.01781) | -1 | -1 |
| G: -6289.08871 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.67575 HOMO: -6.79468 LUMO: -0.39729 factor:1 | 1 (-2.22135) | -1 | -1 |
| G: -6289.08871 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12556.24724 HOMO: -6.93890 LUMO: 0.43266 factor:1 | 1 (-2.79284) | -1 | -1 |
| G: -6289.08871 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.42998 HOMO: -7.08040 LUMO: -0.85716 factor:1 | 1 (-1.97557) | 1 | 1 |
| G: -6289.08871 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12556.02416 HOMO: -6.70216 LUMO: -1.41499 factor:1 | 1 (-2.56976) | -1 | -1 |
| G: -6289.08871 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.28502 HOMO: -6.63686 LUMO: -0.52790 factor:1 | 1 (-1.83062) | -1 | -1 |
| G: -6289.08871 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.44636 HOMO: -6.75114 LUMO: -0.13334 factor:1 | 1 (-1.99196) | -1 | -1 |
| G: -6289.08871 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.29955 HOMO: -6.94435 LUMO: -0.24490 factor:1 | 1 (-1.84515) | -1 | -1 |
| G: -6289.08871 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.13996 HOMO: -6.74298 LUMO: -0.84627 factor:1 | 1 (-1.68555) | -1 | -1 |
| G: -6289.08871 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.45069 HOMO: -7.15932 LUMO: 0.22041 factor:1 | 1 (-0.99629) | 1 | 1 |
| G: -6289.08871 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.28729 HOMO: -6.90081 LUMO: -1.16737 factor:1 | 1 (-0.83289) | -1 | -1 |
| G: -6289.08871 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.28609 HOMO: -7.04775 LUMO: -0.84355 factor:1 | 1 (-0.83169) | -1 | -1 |
| G: -6289.08871 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.41619 HOMO: -7.17020 LUMO: -1.31159 factor:1 | 1 (-0.96179) | 1 | 1 |
| G: -6289.08871 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.45989 HOMO: -7.14571 LUMO: -0.46259 factor:1 | 1 (-1.00549) | 1 | 1 |
| G: -6289.08871 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.17227 HOMO: -7.45048 LUMO: -0.91158 factor:1 | 1 (-0.71786) | 1 | 1 |
| G: -6289.08871 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.18378 HOMO: -6.87360 LUMO: -0.82995 factor:1 | 1 (-0.72937) | -1 | -1 |
| G: -6289.08871 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.42408 HOMO: -7.43415 LUMO: -0.65307 factor:1 | 1 (-0.96968) | 1 | 1 |
| G: -6289.08871 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.23956 HOMO: -7.47225 LUMO: -0.77280 factor:1 | 1 (-0.78516) | 1 | 1 |
| G: -6289.08871 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.01452 HOMO: -6.86271 LUMO: -0.83811 factor:1 | 1 (-0.56012) | -1 | -1 |
| G: -6289.08871 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.36002 HOMO: -7.53483 LUMO: -0.66124 factor:1 | 1 (-0.90562) | 1 | 1 |
| G: -6289.08871 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.24974 HOMO: -7.45864 LUMO: -1.08301 factor:1 | 1 (-0.79533) | 1 | 1 |
| G: -6289.08871 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.69458 HOMO: -7.24639 LUMO: -1.19186 factor:1 | 1 (-2.24018) | 1 | 1 |
| G: -6289.08871 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12556.54091 HOMO: -7.54844 LUMO: -0.96873 factor:1 | 1 (-3.08651) | 1 | 1 |
| G: -6289.08871 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.47561 HOMO: -7.12666 LUMO: -0.01633 factor:1 | 1 (-2.02121) | 1 | 1 |
| G: -6289.08871 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.17578 HOMO: -6.77291 LUMO: -0.70477 factor:1 | 1 (-0.72137) | -1 | -1 |
| G: -6289.08871 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.32821 HOMO: -6.76475 LUMO: -1.15921 factor:1 | 1 (-0.87381) | -1 | -1 |
| G: -6289.08871 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.30291 HOMO: -5.37697 LUMO: -0.56600 factor:1 | 1 (-0.84851) | -1 | -1 |
| G: -6289.08871 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.90936 HOMO: -6.62053 LUMO: -1.75513 factor:1 | 1 (-2.45496) | -1 | -1 |
| G: -6289.08871 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.22799 HOMO: -6.60420 LUMO: -1.74697 factor:1 | 1 (-1.77358) | -1 | -1 |
| G: -6289.08871 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.76027 HOMO: -6.84366 LUMO: -0.94968 factor:1 | 1 (-2.30587) | -1 | -1 |
| G: -6289.08871 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.15008 HOMO: -6.96884 LUMO: -2.11977 factor:1 | 1 (-1.69568) | -1 | -1 |
| G: -6289.08871 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.30859 HOMO: -6.80829 LUMO: 0.56055 factor:1 | 1 (-1.85418) | -1 | -1 |
| G: -6289.08871 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12556.02985 HOMO: -7.02326 LUMO: 0.11429 factor:1 | 1 (-2.57545) | -1 | -1 |
| G: -6289.08871 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.39613 HOMO: -7.40966 LUMO: 0.18232 factor:1 | 1 (-1.94172) | 1 | 1 |
| G: -6289.08871 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12556.18607 HOMO: -6.34570 LUMO: 0.41089 factor:1 | 1 (-2.73167) | -1 | -1 |
| G: -6289.08871 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.23756 HOMO: -6.78924 LUMO: 0.49525 factor:1 | 1 (-1.78316) | -1 | -1 |
| G: -6289.08871 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.66379 HOMO: -6.87632 LUMO: 0.44082 factor:1 | 1 (-1.20938) | -1 | -1 |
| G: -6289.08871 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.52811 HOMO: -6.69944 LUMO: 1.20546 factor:1 | 1 (-1.07371) | -1 | -1 |
| G: -6289.08871 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.71554 HOMO: -6.83006 LUMO: 1.28982 factor:1 | 1 (-1.26114) | -1 | -1 |
| G: -6289.08871 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.53162 HOMO: -7.78246 LUMO: 0.20681 factor:1 | 1 (-1.07722) | 1 | 1 |
| G: -6289.08871 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.36748 HOMO: -6.55794 LUMO: -1.65173 factor:1 | 1 (-0.91308) | -1 | -1 |
| G: -6289.08871 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.70226 HOMO: -6.77564 LUMO: -1.14560 factor:1 | 1 (-1.24786) | -1 | -1 |
| G: -6289.08871 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.97987 HOMO: -7.46680 LUMO: -1.18097 factor:1 | 1 (-1.52547) | 1 | 1 |
| G: -6289.08871 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.93024 HOMO: -6.88176 LUMO: -1.24900 factor:1 | 1 (-1.47584) | -1 | -1 |
| G: -6289.08871 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.80942 HOMO: -7.28177 LUMO: -0.42178 factor:1 | 1 (-1.35502) | 1 | 1 |
| G: -6289.08871 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.43570 HOMO: -7.71715 LUMO: 0.19592 factor:1 | 1 (-0.98130) | 1 | 1 |
| G: -6289.08871 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.96667 HOMO: -7.02326 LUMO: -1.40683 factor:1 | 1 (-1.51227) | -1 | -1 |
| G: -6289.08871 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.70354 HOMO: -7.27088 LUMO: -1.07485 factor:1 | 1 (-1.24914) | 1 | 1 |
| G: -6289.08871 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.84681 HOMO: -7.17020 LUMO: -0.49525 factor:1 | 1 (-1.39241) | 1 | 1 |
| G: -6289.08871 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.75056 HOMO: -7.15932 LUMO: 0.02721 factor:1 | 1 (-1.29616) | 1 | 1 |
| G: -6289.08871 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.85497 HOMO: -7.00693 LUMO: -0.83267 factor:1 | 1 (-1.40057) | -1 | -1 |
| G: -6289.08871 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.87220 HOMO: -6.86543 LUMO: -0.10340 factor:1 | 1 (-1.41779) | -1 | -1 |
| G: -6289.08871 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.69236 HOMO: -7.11850 LUMO: -0.08980 factor:1 | 1 (-1.23795) | 1 | 1 |
| G: -6289.08871 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.53344 HOMO: -6.87087 LUMO: -0.88981 factor:1 | 1 (-1.07904) | -1 | -1 |
| G: -6289.08871 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.70104 HOMO: -7.08857 LUMO: -1.27077 factor:1 | 1 (-1.24664) | 1 | 1 |
| G: -6289.08871 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.68400 HOMO: -6.79468 LUMO: -0.81906 factor:1 | 1 (-1.22960) | -1 | -1 |
| G: -6289.08871 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.37143 HOMO: -6.86815 LUMO: -0.89798 factor:1 | 1 (-0.91702) | -1 | -1 |
| G: -6289.08871 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.71546 HOMO: -6.78652 LUMO: -2.00548 factor:1 | 1 (-1.26106) | -1 | -1 |
| G: -6289.08871 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.74888 HOMO: -6.75114 LUMO: -0.08436 factor:1 | 1 (-1.29447) | -1 | -1 |
| G: -6289.08871 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.37329 HOMO: -6.55794 LUMO: 0.52790 factor:1 | 1 (-1.91889) | -1 | -1 |
| G: -6289.08871 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.41319 HOMO: -7.17836 LUMO: 0.28300 factor:1 | 1 (-1.95878) | 1 | -1 |
| G: -6289.08871 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.61496 HOMO: -7.35796 LUMO: -0.77552 factor:1 | 1 (-2.16056) | 1 | 1 |
| G: -6289.08871 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.59529 HOMO: -7.23551 LUMO: -1.17553 factor:1 | 1 (-2.14088) | 1 | 1 |
| G: -6289.08871 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.52426 HOMO: -7.07496 LUMO: -1.14288 factor:1 | 1 (-2.06986) | 1 | 1 |
| G: -6289.08871 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.46176 HOMO: -6.70489 LUMO: -0.83539 factor:1 | 1 (-2.00736) | -1 | -1 |
| G: -6289.08871 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.80063 HOMO: -6.59604 LUMO: -0.89798 factor:1 | 1 (-1.34623) | -1 | -1 |
| G: -6289.08871 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.93165 HOMO: -6.94162 LUMO: -1.22451 factor:1 | 1 (-1.47725) | -1 | -1 |
| G: -6289.08871 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.79171 HOMO: -6.68040 LUMO: 0.22041 factor:1 | 1 (-1.33730) | -1 | -1 |
| G: -6289.08871 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.04488 HOMO: -6.88176 LUMO: 0.11157 factor:1 | 1 (-1.59048) | -1 | -1 |
| G: -6289.08871 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.32366 HOMO: -6.91713 LUMO: 1.27621 factor:1 | 1 (-1.86926) | -1 | -1 |
| G: -6289.08871 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.24480 HOMO: -6.77836 LUMO: 1.01226 factor:1 | 1 (-1.79040) | -1 | -1 |
| G: -6289.08871 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.30709 HOMO: -7.14571 LUMO: 1.48574 factor:1 | 1 (-1.85269) | 1 | 1 |
| G: -6289.08871 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.36823 HOMO: -6.96884 LUMO: 1.48574 factor:1 | 1 (-1.91383) | -1 | -1 |
| G: -6289.08871 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.25479 HOMO: -7.24367 LUMO: 1.28438 factor:1 | 1 (-1.80039) | 1 | 1 |
| G: -6289.08871 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.98858 HOMO: -7.10489 LUMO: 1.29526 factor:1 | 1 (-1.53418) | 1 | 1 |
| G: -6289.08871 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.49531 HOMO: -7.07224 LUMO: 1.29254 factor:1 | 1 (-2.04091) | 1 | 1 |
| G: -6289.08871 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.42979 HOMO: -7.12938 LUMO: 0.49253 factor:1 | 1 (-1.97538) | 1 | 1 |
| G: -6289.08871 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.28491 HOMO: -7.33619 LUMO: 1.45581 factor:1 | 1 (-1.83051) | 1 | 1 |
| G: -6289.08871 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.09043 HOMO: -6.87904 LUMO: -0.14422 factor:1 | 1 (-1.63603) | -1 | -1 |
| G: -6289.08871 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.10589 HOMO: -6.81917 LUMO: 0.50341 factor:1 | 1 (-1.65149) | -1 | -1 |
| G: -6289.08871 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.33610 HOMO: -7.27905 LUMO: 0.13606 factor:1 | 1 (-1.88169) | 1 | -1 |
| G: -6289.08871 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.36807 HOMO: -6.87904 LUMO: -0.09796 factor:1 | 1 (-1.91367) | -1 | -1 |
| G: -6289.08871 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.10679 HOMO: -7.33891 LUMO: 0.03810 factor:1 | 1 (-1.65238) | 1 | 1 |
| G: -6289.08871 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.94224 HOMO: -6.98516 LUMO: 0.98233 factor:1 | 1 (-1.48784) | -1 | -1 |
| G: -6289.08871 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.29370 HOMO: -6.94162 LUMO: 0.86804 factor:1 | 1 (-1.83930) | -1 | -1 |
| G: -6289.08871 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.35142 HOMO: -7.37701 LUMO: 0.05442 factor:1 | 1 (-1.89701) | 1 | 1 |
| G: -6289.08871 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.63042 HOMO: -7.04775 LUMO: 0.43266 factor:1 | 1 (-1.17602) | -1 | -1 |
| G: -6289.08871 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.56806 HOMO: -7.47497 LUMO: 0.31837 factor:1 | 1 (-1.11365) | 1 | 1 |
| G: -6289.08871 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.39341 HOMO: -6.62053 LUMO: 0.13061 factor:1 | 1 (-0.93901) | -1 | -1 |
| G: -6289.08871 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.21458 HOMO: -6.44366 LUMO: -0.04354 factor:1 | 1 (-0.76018) | -1 | -1 |
| G: -6289.08871 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.14043 HOMO: -6.40284 LUMO: 0.68301 factor:1 | 1 (-0.68603) | -1 | -1 |
| G: -6289.08871 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.77296 HOMO: -6.73754 LUMO: 0.36735 factor:1 | 1 (-1.31855) | -1 | -1 |
| G: -6289.08871 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.45850 HOMO: -6.85455 LUMO: 0.23946 factor:1 | 1 (-1.00410) | -1 | -1 |
| G: -6289.08871 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.61687 HOMO: -6.93346 LUMO: 0.24762 factor:1 | 1 (-1.16247) | -1 | -1 |
| G: -6289.08871 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.70006 HOMO: -6.85455 LUMO: 0.17687 factor:1 | 1 (-1.24566) | -1 | -1 |
| G: -6289.08871 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.50748 HOMO: -6.62325 LUMO: 0.69933 factor:1 | 1 (-1.05308) | -1 | -1 |
| G: -6289.08871 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.34389 HOMO: -6.43005 LUMO: 0.50069 factor:1 | 1 (-0.88949) | -1 | -1 |
| G: -6289.08871 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.59108 HOMO: -6.56883 LUMO: 0.22858 factor:1 | 1 (-1.13667) | -1 | -1 |
| G: -6289.08871 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.49173 HOMO: -6.78380 LUMO: 0.54967 factor:1 | 1 (-1.03733) | -1 | -1 |
| G: -6289.08871 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.62348 HOMO: -7.35524 LUMO: 0.00272 factor:1 | 1 (-1.16908) | 1 | 1 |
| G: -6289.08871 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.41907 HOMO: -7.27360 LUMO: 0.08436 factor:1 | 1 (-0.96467) | 1 | 1 |
| G: -6289.08871 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.27417 HOMO: -7.44504 LUMO: -0.96056 factor:1 | 1 (-0.81977) | 1 | 1 |
| G: -6289.08871 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.55823 HOMO: -7.27360 LUMO: 0.29933 factor:1 | 1 (-1.10383) | 1 | 1 |
| G: -6289.08871 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.24412 HOMO: -7.09129 LUMO: 0.41089 factor:1 | 1 (-1.78972) | 1 | 1 |
| G: -6289.08871 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.28050 HOMO: -6.93618 LUMO: 0.36463 factor:1 | 1 (-1.82610) | -1 | -1 |
| G: -6289.08871 HOMO: -7.26000 LUMO: -3.02863 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.20548 HOMO: -7.65728 LUMO: 0.20136 factor:1 | 1 (-1.75108) | 1 | 1 |
| G: -6289.08871 HOMO: -7.26000 LUMO: -3.02863 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.85255 HOMO: -6.90353 LUMO: -0.92791 factor:1 | 1 (-1.39815) | -1 | -1 |
| G: -6289.08871 HOMO: -7.26000 LUMO: -3.02863 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.27327 HOMO: -6.82462 LUMO: -1.18370 factor:1 | 1 (-1.81886) | -1 | -1 |
| G: -6289.08871 HOMO: -7.26000 LUMO: -3.02863 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.07533 HOMO: -7.09129 LUMO: -0.13334 factor:1 | 1 (-1.62093) | 1 | 1 |
| G: -6289.08871 HOMO: -7.26000 LUMO: -3.02863 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.75056 HOMO: -7.40966 LUMO: -1.06941 factor:1 | 1 (-1.29616) | 1 | 1 |
| G: -6289.08871 HOMO: -7.26000 LUMO: -3.02863 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.52359 HOMO: -7.24367 LUMO: -1.00954 factor:1 | 1 (-1.06919) | 1 | 1 |
| G: -6289.08871 HOMO: -7.26000 LUMO: -3.02863 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.60291 HOMO: -7.51851 LUMO: 0.09796 factor:1 | 1 (-1.14851) | 1 | 1 |
| G: -6289.08871 HOMO: -7.26000 LUMO: -3.02863 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.25371 HOMO: -7.48857 LUMO: -0.07619 factor:1 | 1 (-0.79931) | 1 | 1 |
| G: -6289.08871 HOMO: -7.26000 LUMO: -3.02863 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.67540 HOMO: -6.53345 LUMO: 1.09390 factor:1 | 1 (-1.22100) | -1 | -1 |
| G: -6289.08871 HOMO: -7.26000 LUMO: -3.02863 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.34794 HOMO: -7.21918 LUMO: 0.08436 factor:1 | 1 (-0.89354) | 1 | 1 |
| G: -6289.08871 HOMO: -7.26000 LUMO: -3.02863 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.19618 HOMO: -7.38789 LUMO: 1.02587 factor:1 | 1 (-0.74178) | 1 | -1 |
| G: -6289.08871 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.47156 HOMO: -6.83550 LUMO: -0.67484 factor:1 | 1 (-1.01716) | -1 | -1 |
| G: -6289.08871 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.44552 HOMO: -7.04231 LUMO: 0.54151 factor:1 | 1 (-0.99112) | -1 | -1 |
| G: -6289.08871 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.63059 HOMO: -6.79740 LUMO: 1.91296 factor:1 | 1 (-1.17618) | 1 | 1 |
| G: -6289.08871 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.74634 HOMO: -7.35796 LUMO: -1.04220 factor:1 | 1 (-1.29194) | -1 | -1 |
| G: -6289.08871 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.83247 HOMO: -6.62597 LUMO: -0.44082 factor:1 | 1 (-1.37807) | -1 | -1 |
| G: -6289.08871 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.58528 HOMO: -6.45182 LUMO: -0.20409 factor:1 | 1 (-1.13088) | -1 | -1 |
| G: -6289.08871 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.54672 HOMO: -6.51168 LUMO: -0.23130 factor:1 | 1 (-1.09232) | -1 | -1 |
| G: -6289.08871 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.42247 HOMO: -7.14027 LUMO: 0.49797 factor:1 | 1 (-0.96807) | -1 | -1 |
| G: -6289.08871 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.54158 HOMO: -7.55660 LUMO: 0.24762 factor:1 | 1 (-1.08718) | -1 | -1 |
| G: -6289.08871 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.55548 HOMO: -6.88992 LUMO: -0.64763 factor:1 | 1 (-1.10108) | -1 | -1 |
| G: -6289.08871 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.29717 HOMO: -6.72665 LUMO: -0.45987 factor:1 | 1 (-0.84276) | -1 | -1 |
| G: -6289.08871 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.61508 HOMO: -6.72121 LUMO: -0.58232 factor:1 | 1 (-1.16067) | -1 | -1 |
| G: -6289.08871 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.26838 HOMO: -7.26816 LUMO: 0.32926 factor:1 | 1 (-0.81397) | -1 | -1 |
| G: -6289.08871 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.37134 HOMO: -6.57155 LUMO: -0.53606 factor:1 | 1 (-0.91694) | -1 | -1 |
| G: -6289.08871 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.18625 HOMO: -6.50896 LUMO: -0.43810 factor:1 | 1 (-0.73185) | -1 | -1 |
| G: -6289.08871 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.00451 HOMO: -6.73210 LUMO: -0.51430 factor:1 | 1 (-0.55011) | -1 | -1 |
| G: -6289.08871 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.50678 HOMO: -6.77019 LUMO: -0.62858 factor:1 | 1 (-1.05237) | -1 | -1 |
| G: -6289.08871 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.17507 HOMO: -6.82462 LUMO: -0.67484 factor:1 | 1 (-0.72067) | -1 | -1 |
| G: -6289.08871 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.76575 HOMO: -6.79740 LUMO: -0.55511 factor:1 | 1 (-1.31134) | -1 | -1 |
| G: -6289.08871 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.65780 HOMO: -6.79740 LUMO: -0.67756 factor:1 | 1 (-1.20340) | -1 | -1 |
| G: -6289.08871 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.14975 HOMO: -6.75114 LUMO: -0.55239 factor:1 | 1 (-1.69535) | -1 | -1 |
| G: -6289.08871 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.18023 HOMO: -6.49536 LUMO: -0.25307 factor:1 | 1 (-1.72583) | -1 | -1 |
| G: -6289.08871 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.04140 HOMO: -6.48992 LUMO: -0.25034 factor:1 | 1 (-1.58700) | -1 | -1 |
| G: -6289.08871 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.36113 HOMO: -6.52801 LUMO: -0.28028 factor:1 | 1 (-1.90673) | -1 | -1 |
| G: -6289.08871 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.41039 HOMO: -7.22462 LUMO: 0.52518 factor:1 | 1 (-0.95599) | -1 | -1 |
| G: -6289.08871 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.26166 HOMO: -6.59332 LUMO: -0.27211 factor:1 | 1 (-0.80725) | -1 | -1 |
| G: -6289.08871 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12553.97194 HOMO: -6.57427 LUMO: -0.16871 factor:1 | 1 (-0.51753) | -1 | -1 |
| G: -6289.08871 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.07330 HOMO: -6.71033 LUMO: 1.59187 factor:1 | 1 (-0.61890) | 1 | 1 |
| G: -6289.08871 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12553.76902 HOMO: -6.72121 LUMO: 2.00004 factor:1 | 1 (-0.31462) | 1 | 1 |
| G: -6289.08871 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12553.41067 HOMO: -6.61509 LUMO: 1.55921 factor:1 | -1 (0.04373) | -1 | -1 |
| G: -6289.08871 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.17548 HOMO: -6.55250 LUMO: 1.73064 factor:1 | 1 (-0.72107) | -1 | -1 |
| G: -6289.08871 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.85171 HOMO: -6.66135 LUMO: 2.02181 factor:1 | 1 (-1.39730) | 1 | 1 |
| G: -6289.08871 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.72523 HOMO: -6.84911 LUMO: 1.98099 factor:1 | 1 (-1.27083) | 1 | 1 |
| G: -6289.08871 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.63233 HOMO: -6.66679 LUMO: 1.98371 factor:1 | 1 (-1.17793) | 1 | 1 |
| G: -6289.08871 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.82349 HOMO: -6.67495 LUMO: 2.04085 factor:1 | 1 (-1.36909) | 1 | 1 |
| G: -6289.08871 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.54321 HOMO: -6.89809 LUMO: 1.95106 factor:1 | 1 (-1.08881) | 1 | 1 |
| G: -6289.08871 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.64433 HOMO: -6.50352 LUMO: 1.88847 factor:1 | 1 (-1.18993) | -1 | -1 |
| G: -6289.08871 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.39890 HOMO: -6.93618 LUMO: 2.00004 factor:1 | 1 (-1.94450) | 1 | 1 |
| G: -6289.08871 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.51724 HOMO: -6.50896 LUMO: 1.73609 factor:1 | 1 (-2.06284) | -1 | -1 |
| G: -6289.08871 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.55733 HOMO: -6.69672 LUMO: 2.37283 factor:1 | 1 (-2.10292) | 1 | 1 |
| G: -6289.08871 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.30592 HOMO: -6.65591 LUMO: 2.20684 factor:1 | 1 (-1.85152) | 1 | 1 |
| G: -6289.08871 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.35501 HOMO: -6.23957 LUMO: 1.78507 factor:1 | 1 (-1.90061) | -1 | -1 |
| G: -6289.08871 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.73402 HOMO: -6.35114 LUMO: 1.92112 factor:1 | 1 (-1.27962) | -1 | -1 |
| G: -6289.08871 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.80036 HOMO: -6.53617 LUMO: 1.75241 factor:1 | 1 (-1.34596) | -1 | -1 |
| G: -6289.08871 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.63363 HOMO: -6.60420 LUMO: 1.78779 factor:1 | 1 (-1.17923) | 1 | 1 |
| G: -6289.08871 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.52204 HOMO: -7.40422 LUMO: -0.97145 factor:1 | 1 (-1.06764) | -1 | -1 |
| G: -6289.08871 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.42841 HOMO: -6.80013 LUMO: -0.69117 factor:1 | 1 (-0.97400) | -1 | -1 |
| G: -6289.08871 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.35205 HOMO: -6.68040 LUMO: -0.47076 factor:1 | 1 (-0.89765) | -1 | -1 |
| G: -6289.08871 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.38996 HOMO: -7.20285 LUMO: -0.66124 factor:1 | 1 (-0.93555) | -1 | -1 |
| G: -6289.08871 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.11594 HOMO: -6.82734 LUMO: -0.60137 factor:1 | 1 (-0.66154) | -1 | -1 |
| G: -6289.08871 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.48307 HOMO: -7.18653 LUMO: 0.59321 factor:1 | 1 (-1.02867) | -1 | -1 |
| G: -6289.08871 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.35400 HOMO: -7.29265 LUMO: 0.48164 factor:1 | 1 (-1.89960) | -1 | -1 |
| G: -6289.08871 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.54952 HOMO: -6.63414 LUMO: -0.25034 factor:1 | 1 (-2.09511) | -1 | -1 |
| G: -6289.08871 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.08924 HOMO: -7.20285 LUMO: 0.53879 factor:1 | 1 (-1.63483) | -1 | -1 |
| G: -6289.08871 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.51860 HOMO: -6.46815 LUMO: -0.21769 factor:1 | 1 (-2.06420) | -1 | -1 |
| G: -6289.08871 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.36355 HOMO: -6.57971 LUMO: -0.18776 factor:1 | 1 (-1.90915) | -1 | -1 |
| G: -6289.08871 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.80575 HOMO: -6.90897 LUMO: 1.91296 factor:1 | 1 (-1.35134) | 1 | 1 |
| G: -6289.08871 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.54626 HOMO: -6.67495 LUMO: 2.04358 factor:1 | 1 (-1.09186) | 1 | 1 |
| G: -6289.08871 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.68245 HOMO: -6.94162 LUMO: 1.73881 factor:1 | 1 (-1.22805) | 1 | 1 |
| G: -6289.08871 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.37311 HOMO: -6.73482 LUMO: 1.95922 factor:1 | 1 (-0.91871) | 1 | 1 |
| G: -6289.08871 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.17839 HOMO: -6.70489 LUMO: 2.04358 factor:1 | 1 (-0.72399) | 1 | 1 |
| G: -6289.08871 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.39826 HOMO: -7.04231 LUMO: 1.79323 factor:1 | 1 (-0.94385) | 1 | 1 |
| G: -6289.08871 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.60539 HOMO: -6.68584 LUMO: 1.60275 factor:1 | 1 (-1.15099) | 1 | 1 |
| G: -6289.08871 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.75625 HOMO: -6.40556 LUMO: 1.45581 factor:1 | 1 (-1.30185) | -1 | -1 |
| G: -6289.08871 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.44792 HOMO: -6.94979 LUMO: 2.16603 factor:1 | 1 (-0.99351) | 1 | 1 |
| G: -6289.08871 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.55932 HOMO: -6.84911 LUMO: 1.89935 factor:1 | 1 (-1.10492) | 1 | 1 |
| G: -6289.08871 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.62261 HOMO: -6.22052 LUMO: 1.57282 factor:1 | 1 (-1.16821) | -1 | -1 |
| G: -6289.08871 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.19605 HOMO: -6.51168 LUMO: 2.10072 factor:1 | 1 (-0.74165) | -1 | -1 |
| G: -6289.08871 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.19891 HOMO: -7.03686 LUMO: 2.12249 factor:1 | 1 (-0.74450) | 1 | 1 |
| G: -6289.08871 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12553.93044 HOMO: -6.84094 LUMO: 1.63268 factor:1 | 1 (-0.47604) | 1 | 1 |
| G: -6289.08871 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.33929 HOMO: -6.75387 LUMO: 1.72248 factor:1 | 1 (-0.88489) | 1 | 1 |
| G: -6289.08871 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.55102 HOMO: -6.86271 LUMO: 1.68711 factor:1 | 1 (-1.09662) | 1 | 1 |
| G: -6289.08871 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.54346 HOMO: -6.84094 LUMO: 2.02997 factor:1 | 1 (-1.08905) | 1 | 1 |
| G: -6289.08871 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.52451 HOMO: -6.80557 LUMO: 2.02725 factor:1 | 1 (-2.07011) | 1 | 1 |
| G: -6289.08871 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.58799 HOMO: -6.38651 LUMO: 1.53472 factor:1 | 1 (-2.13359) | -1 | -1 |
| G: -6289.08871 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.34230 HOMO: -7.51306 LUMO: 0.28572 factor:1 | 1 (-1.88790) | -1 | -1 |
| G: -6289.08871 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.37732 HOMO: -6.97972 LUMO: -0.74287 factor:1 | 1 (-1.92292) | -1 | -1 |
| G: -6289.08871 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.20799 HOMO: -6.83822 LUMO: -0.65852 factor:1 | 1 (-1.75358) | -1 | -1 |
| G: -6289.08871 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.24102 HOMO: -6.71305 LUMO: -0.49525 factor:1 | 1 (-1.78662) | -1 | -1 |
| G: -6289.08871 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.19558 HOMO: -6.60692 LUMO: -0.22313 factor:1 | 1 (-1.74117) | -1 | -1 |
| G: -6289.08871 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.38140 HOMO: -7.20013 LUMO: 0.55239 factor:1 | 1 (-1.92700) | -1 | -1 |
| G: -6289.08871 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.28284 HOMO: -6.60420 LUMO: -0.28028 factor:1 | 1 (-1.82844) | -1 | -1 |
| G: -6289.08871 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.01748 HOMO: -6.69128 LUMO: -0.30477 factor:1 | 1 (-1.56308) | -1 | -1 |
| G: -6289.08871 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.35865 HOMO: -6.65591 LUMO: -0.25579 factor:1 | 1 (-1.90425) | -1 | -1 |
| G: -6289.08871 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.25729 HOMO: -6.69128 LUMO: 1.70888 factor:1 | 1 (-1.80289) | 1 | 1 |
| G: -6289.08871 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.27884 HOMO: -6.50080 LUMO: 1.87759 factor:1 | 1 (-1.82444) | -1 | -1 |
| G: -6289.08871 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.10858 HOMO: -6.85727 LUMO: 1.99187 factor:1 | 1 (-1.65418) | 1 | 1 |
| G: -6289.08871 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.32355 HOMO: -6.58788 LUMO: 1.79051 factor:1 | 1 (-1.86915) | 1 | 1 |
| G: -6289.08871 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.35972 HOMO: -6.64230 LUMO: 2.16058 factor:1 | 1 (-1.90531) | 1 | 1 |
| G: -6289.08871 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.51466 HOMO: -6.58788 LUMO: 2.10616 factor:1 | 1 (-2.06026) | 1 | 1 |
| G: -6289.08871 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.34935 HOMO: -7.01782 LUMO: 2.13609 factor:1 | 1 (-1.89495) | 1 | 1 |
| G: -6289.08871 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.16924 HOMO: -6.31304 LUMO: 2.31841 factor:1 | 1 (-1.71483) | -1 | -1 |
| G: -6289.08871 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.10091 HOMO: -6.94979 LUMO: 2.07895 factor:1 | 1 (-1.64651) | 1 | 1 |
| G: -6289.08871 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.39294 HOMO: -6.88992 LUMO: 2.28031 factor:1 | 1 (-1.93854) | 1 | 1 |
| G: -6289.08871 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.40271 HOMO: -6.66407 LUMO: 2.07623 factor:1 | 1 (-1.94831) | 1 | 1 |
| G: -6289.08871 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.43825 HOMO: -6.52529 LUMO: 1.70071 factor:1 | 1 (-1.98385) | -1 | -1 |
| G: -6289.08871 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.23220 HOMO: -6.58788 LUMO: 1.57282 factor:1 | 1 (-1.77780) | -1 | -1 |
| G: -6289.08871 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.40211 HOMO: -6.55250 LUMO: 1.95378 factor:1 | 1 (-1.94771) | -1 | -1 |
| G: -6289.08871 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.02986 HOMO: -6.24773 LUMO: 1.77962 factor:1 | 1 (-1.57546) | -1 | -1 |
| G: -6289.08871 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.99214 HOMO: -6.31304 LUMO: 2.18507 factor:1 | 1 (-1.53774) | -1 | -1 |
| G: -6289.08871 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.32070 HOMO: -6.18243 LUMO: 2.01636 factor:1 | 1 (-1.86629) | -1 | -1 |
| G: -6289.08871 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.17234 HOMO: -6.99877 LUMO: 2.14970 factor:1 | 1 (-1.71794) | 1 | 1 |
| G: -6289.08871 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.45336 HOMO: -6.72665 LUMO: 2.07079 factor:1 | 1 (-0.99896) | 1 | 1 |
| G: -6289.08871 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.56604 HOMO: -6.36202 LUMO: 2.17419 factor:1 | 1 (-1.11164) | -1 | -1 |
| G: -6289.08871 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.59407 HOMO: -6.78652 LUMO: 2.05718 factor:1 | 1 (-1.13967) | 1 | -1 |
| G: -6289.08871 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.70833 HOMO: -6.87360 LUMO: 2.34290 factor:1 | 1 (-1.25393) | 1 | 1 |
| G: -6289.08871 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.32947 HOMO: -6.62053 LUMO: 1.89391 factor:1 | 1 (-0.87506) | 1 | 1 |
| G: -6289.08871 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.38666 HOMO: -6.58788 LUMO: 1.83133 factor:1 | 1 (-0.93226) | 1 | 1 |
| G: -6289.08871 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.43706 HOMO: -7.08584 LUMO: 1.91568 factor:1 | 1 (-0.98266) | 1 | 1 |
| G: -6289.08871 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.62566 HOMO: -6.56883 LUMO: 1.81228 factor:1 | 1 (-1.17126) | 1 | 1 |
| G: -6289.08871 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.51948 HOMO: -6.66135 LUMO: 1.92384 factor:1 | 1 (-1.06508) | 1 | 1 |
| G: -6289.08871 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.48922 HOMO: -6.64502 LUMO: 2.15786 factor:1 | 1 (-1.03482) | 1 | 1 |
| G: -6289.08871 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.33834 HOMO: -6.71305 LUMO: 1.91840 factor:1 | 1 (-0.88393) | 1 | 1 |
| G: -6289.08871 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.45330 HOMO: -6.44094 LUMO: 1.74425 factor:1 | 1 (-1.99889) | -1 | -1 |
| G: -6289.08871 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.46927 HOMO: -6.51985 LUMO: 1.84221 factor:1 | 1 (-2.01487) | -1 | -1 |
| G: -6289.08871 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.21560 HOMO: -6.63414 LUMO: -0.24762 factor:1 | 1 (-1.76120) | -1 | -1 |
| G: -6289.08871 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.54524 HOMO: -6.60420 LUMO: -0.22585 factor:1 | 1 (-2.09084) | -1 | -1 |
| G: -6289.08871 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.30859 HOMO: -7.19741 LUMO: 0.58232 factor:1 | 1 (-1.85418) | -1 | -1 |
| G: -6289.08871 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.15718 HOMO: -6.77019 LUMO: -0.56872 factor:1 | 1 (-1.70278) | -1 | -1 |
| G: -6289.08871 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.97383 HOMO: -7.46136 LUMO: 0.28844 factor:1 | 1 (-1.51943) | -1 | -1 |
| G: -6289.08871 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.38042 HOMO: -6.60420 LUMO: -0.54151 factor:1 | 1 (-1.92602) | -1 | -1 |
| G: -6289.08871 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.17073 HOMO: -6.53890 LUMO: -0.46531 factor:1 | 1 (-1.71633) | -1 | -1 |
| G: -6289.08871 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.34355 HOMO: -6.81645 LUMO: -0.57144 factor:1 | 1 (-1.88915) | -1 | -1 |
| G: -6289.08871 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.29865 HOMO: -7.48041 LUMO: 0.28572 factor:1 | 1 (-1.84425) | -1 | -1 |
| G: -6289.08871 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.10551 HOMO: -6.75659 LUMO: -0.45715 factor:1 | 1 (-1.65111) | -1 | -1 |
| G: -6289.08871 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.00766 HOMO: -6.66135 LUMO: -0.41906 factor:1 | 1 (-1.55325) | -1 | -1 |
| G: -6289.08871 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.39501 HOMO: -6.55794 LUMO: -0.27483 factor:1 | 1 (-1.94061) | -1 | -1 |
| G: -6289.08871 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.25174 HOMO: -7.07496 LUMO: -0.63403 factor:1 | 1 (-1.79734) | -1 | -1 |
| G: -6289.08871 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.95043 HOMO: -7.12394 LUMO: 0.53334 factor:1 | 1 (-1.49603) | -1 | -1 |
| G: -6289.08871 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.90599 HOMO: -6.53617 LUMO: -0.25579 factor:1 | 1 (-1.45159) | -1 | -1 |
| G: -6289.08871 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.79331 HOMO: -6.50896 LUMO: -0.25034 factor:1 | 1 (-1.33891) | -1 | -1 |
| G: -6289.08871 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.46476 HOMO: -7.17564 LUMO: -0.68573 factor:1 | 1 (-1.01036) | -1 | -1 |
| G: -6289.08871 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.19547 HOMO: -6.53617 LUMO: -0.30749 factor:1 | 1 (-1.74107) | -1 | -1 |
| G: -6289.08871 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.06020 HOMO: -6.55522 LUMO: -0.30749 factor:1 | 1 (-1.60580) | -1 | -1 |
| G: -6289.08871 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.85639 HOMO: -7.05591 LUMO: -0.71022 factor:1 | 1 (-1.40199) | -1 | -1 |
| G: -6289.08871 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.24048 HOMO: -7.17564 LUMO: -0.69933 factor:1 | 1 (-1.78607) | -1 | -1 |
| G: -6289.08871 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.06317 HOMO: -6.78380 LUMO: -0.67756 factor:1 | 1 (-1.60876) | -1 | -1 |
| G: -6289.08871 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.20154 HOMO: -6.62325 LUMO: 2.02725 factor:1 | 1 (-1.74713) | 1 | 1 |
| G: -6289.08871 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.41819 HOMO: -6.63414 LUMO: 1.91296 factor:1 | 1 (-1.96379) | 1 | -1 |
| G: -6289.08871 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.97078 HOMO: -6.83278 LUMO: 1.65717 factor:1 | 1 (-1.51638) | 1 | 1 |
| G: -6289.08871 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.90708 HOMO: -6.66407 LUMO: 1.95650 factor:1 | 1 (-1.45268) | 1 | 1 |
| G: -6289.08871 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.99133 HOMO: -6.61237 LUMO: 2.11432 factor:1 | 1 (-1.53693) | 1 | 1 |
| G: -6289.08871 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.35686 HOMO: -6.62053 LUMO: 2.09256 factor:1 | 1 (-1.90246) | 1 | -1 |
| G: -6289.08871 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.15615 HOMO: -6.78652 LUMO: 2.13609 factor:1 | 1 (-1.70175) | 1 | 1 |
| G: -6289.08871 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.22790 HOMO: -6.94707 LUMO: 1.81772 factor:1 | 1 (-1.77350) | 1 | 1 |
| G: -6289.08871 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.13960 HOMO: -6.85183 LUMO: 2.12793 factor:1 | 1 (-1.68520) | 1 | 1 |
| G: -6289.08871 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.36355 HOMO: -6.81101 LUMO: 1.83949 factor:1 | 1 (-1.90915) | 1 | 1 |
| G: -6289.08871 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.86058 HOMO: -6.98788 LUMO: 2.16058 factor:1 | 1 (-1.40618) | 1 | 1 |
| G: -6289.08871 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.73361 HOMO: -6.62869 LUMO: 2.00820 factor:1 | 1 (-1.27921) | 1 | 1 |
| G: -6289.08871 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.83489 HOMO: -6.34025 LUMO: 2.25855 factor:1 | 1 (-1.38049) | -1 | -1 |
| G: -6289.08871 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.46999 HOMO: -6.01372 LUMO: 2.01636 factor:1 | 1 (-1.01558) | -1 | -1 |
| G: -6289.08871 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.11628 HOMO: -6.89264 LUMO: 2.27487 factor:1 | 1 (-1.66188) | 1 | 1 |
| G: -6289.08871 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.91271 HOMO: -6.53073 LUMO: 2.20684 factor:1 | 1 (-1.45831) | -1 | -1 |
| G: -6289.08871 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.90833 HOMO: -6.83278 LUMO: 1.53744 factor:1 | 1 (-1.45393) | -1 | -1 |
| G: -6289.08871 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.82675 HOMO: -6.41917 LUMO: 1.82316 factor:1 | 1 (-1.37235) | -1 | -1 |
| G: -6289.08871 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.64019 HOMO: -6.56339 LUMO: 1.63813 factor:1 | 1 (-1.18579) | -1 | -1 |
| G: -6289.08871 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.11182 HOMO: -6.88992 LUMO: 1.65173 factor:1 | 1 (-1.65742) | 1 | 1 |
| G: -6289.08871 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.80557 HOMO: -6.63141 LUMO: 1.92112 factor:1 | 1 (-2.35117) | 1 | 1 |
| G: -6289.08871 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12556.58268 HOMO: -6.83822 LUMO: 1.88847 factor:1 | 1 (-3.12828) | 1 | 1 |
| G: -6289.08871 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.45983 HOMO: -6.84638 LUMO: 1.90480 factor:1 | 1 (-2.00542) | 1 | 1 |
| G: -6289.08871 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.60160 HOMO: -6.82462 LUMO: 1.70888 factor:1 | 1 (-2.14720) | 1 | 1 |
| G: -6289.08871 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.80664 HOMO: -6.82734 LUMO: 2.12521 factor:1 | 1 (-2.35223) | 1 | 1 |
| G: -6289.08871 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.39713 HOMO: -6.94435 LUMO: 1.87214 factor:1 | 1 (-1.94273) | 1 | 1 |
| G: -6289.08871 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.89643 HOMO: -6.98516 LUMO: 2.51433 factor:1 | 1 (-2.44203) | 1 | 1 |
| G: -6289.08871 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12556.40423 HOMO: -6.74026 LUMO: 2.15514 factor:1 | 1 (-2.94982) | 1 | 1 |
| G: -6289.08871 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12556.12193 HOMO: -6.93618 LUMO: 2.54426 factor:1 | 1 (-2.66753) | 1 | 1 |
| G: -6289.08871 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12556.58015 HOMO: -6.28583 LUMO: 2.53610 factor:1 | 1 (-3.12574) | -1 | -1 |
| G: -6289.08871 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.42173 HOMO: -6.56883 LUMO: 1.94834 factor:1 | 1 (-1.96733) | 1 | 1 |
| G: -6289.08871 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.23816 HOMO: -7.08584 LUMO: 1.99187 factor:1 | 1 (-1.78376) | 1 | 1 |
| G: -6289.08871 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.05566 HOMO: -6.19059 LUMO: 1.99732 factor:1 | 1 (-1.60125) | -1 | -1 |
| G: -6289.08871 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12556.52153 HOMO: -6.78108 LUMO: 2.03813 factor:1 | 1 (-3.06713) | 1 | 1 |
| G: -6289.08871 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.73961 HOMO: -6.82189 LUMO: 1.77418 factor:1 | 1 (-2.28521) | 1 | 1 |
| G: -6289.08871 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12556.66714 HOMO: -6.45454 LUMO: 1.78779 factor:1 | 1 (-3.21274) | -1 | -1 |
| G: -6289.08871 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.36274 HOMO: -6.84366 LUMO: 1.77690 factor:1 | 1 (-1.90833) | 1 | 1 |
| G: -6289.08871 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12556.13257 HOMO: -6.74026 LUMO: 1.67622 factor:1 | 1 (-2.67817) | 1 | 1 |
| G: -6289.08871 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.88773 HOMO: -6.76475 LUMO: 2.40277 factor:1 | 1 (-2.43332) | 1 | 1 |
| G: -6289.08871 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.67365 HOMO: -6.65863 LUMO: 1.86670 factor:1 | 1 (-2.21925) | 1 | 1 |
| G: -6289.08871 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.52623 HOMO: -6.50080 LUMO: 1.93201 factor:1 | 1 (-1.07183) | -1 | -1 |
| G: -6289.08871 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.39515 HOMO: -6.34842 LUMO: 1.70888 factor:1 | 1 (-0.94075) | -1 | -1 |
| G: -6289.08871 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.93986 HOMO: -6.60692 LUMO: 2.20140 factor:1 | 1 (-2.48546) | 1 | 1 |
| G: -6289.08871 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.39808 HOMO: -6.74026 LUMO: 2.14970 factor:1 | 1 (-1.94368) | 1 | 1 |
| G: -6289.08871 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.79034 HOMO: -6.63686 LUMO: 2.17419 factor:1 | 1 (-2.33593) | 1 | 1 |
| G: -6289.08871 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.34219 HOMO: -6.81917 LUMO: 2.10072 factor:1 | 1 (-1.88779) | 1 | -1 |
| G: -6289.08871 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.28611 HOMO: -6.92802 LUMO: 2.04358 factor:1 | 1 (-1.83171) | 1 | 1 |
| G: -6289.08871 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.39599 HOMO: -6.56067 LUMO: -0.47620 factor:1 | 1 (-1.94159) | -1 | -1 |
| G: -6289.08871 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.31789 HOMO: -6.56611 LUMO: -0.77008 factor:1 | 1 (-1.86349) | -1 | -1 |
| G: -6289.08871 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.45928 HOMO: -6.78380 LUMO: -0.64763 factor:1 | 1 (-2.00488) | -1 | -1 |
| G: -6289.08871 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.24505 HOMO: -6.51985 LUMO: -0.24490 factor:1 | 1 (-1.79065) | -1 | -1 |
| G: -6289.08871 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.11258 HOMO: -6.52529 LUMO: -0.27483 factor:1 | 1 (-1.65818) | -1 | -1 |
| G: -6289.08871 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.18151 HOMO: -7.10489 LUMO: -0.62586 factor:1 | 1 (-1.72711) | -1 | -1 |
| G: -6289.08871 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.89111 HOMO: -7.18108 LUMO: 0.48980 factor:1 | 1 (-1.43671) | -1 | -1 |
| G: -6289.08871 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.63368 HOMO: -7.14299 LUMO: -0.63947 factor:1 | 1 (-2.17928) | -1 | -1 |
| G: -6289.08871 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.82449 HOMO: -6.70761 LUMO: -0.54423 factor:1 | 1 (-2.37008) | -1 | -1 |
| G: -6289.08871 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.62680 HOMO: -7.32258 LUMO: -1.03675 factor:1 | 1 (-2.17239) | -1 | -1 |
| G: -6289.08871 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.85341 HOMO: -6.65046 LUMO: -0.41361 factor:1 | 1 (-2.39901) | -1 | -1 |
| G: -6289.08871 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12556.43340 HOMO: -6.76475 LUMO: -0.60137 factor:1 | 1 (-2.97899) | -1 | -1 |
| G: -6289.08871 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.65975 HOMO: -6.77836 LUMO: -0.54423 factor:1 | 1 (-2.20535) | -1 | -1 |
| G: -6289.08871 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12556.13021 HOMO: -7.52395 LUMO: 0.26395 factor:1 | 1 (-2.67580) | -1 | -1 |
| G: -6289.08871 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12556.21704 HOMO: -6.93890 LUMO: -0.72382 factor:1 | 1 (-2.76264) | -1 | -1 |
| G: -6289.08871 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.49700 HOMO: -6.72938 LUMO: -0.47348 factor:1 | 1 (-2.04260) | -1 | -1 |
| G: -6289.08871 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12556.06212 HOMO: -6.66951 LUMO: -0.40817 factor:1 | 1 (-2.60772) | -1 | -1 |
| G: -6289.08871 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.34369 HOMO: -6.60420 LUMO: -0.19320 factor:1 | 1 (-1.88929) | -1 | -1 |
| G: -6289.08871 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.41808 HOMO: -6.67495 LUMO: -0.27211 factor:1 | 1 (-1.96368) | -1 | -1 |
| G: -6289.08871 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.62152 HOMO: -7.23823 LUMO: -0.62858 factor:1 | 1 (-2.16711) | -1 | -1 |
| G: -6289.08871 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.46562 HOMO: -7.27088 LUMO: 0.53334 factor:1 | 1 (-2.01122) | -1 | -1 |
| G: -6289.08871 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.23713 HOMO: -7.20013 LUMO: 0.59049 factor:1 | 1 (-1.78273) | -1 | -1 |
| G: -6289.08871 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.25264 HOMO: -6.60148 LUMO: -0.20953 factor:1 | 1 (-1.79824) | -1 | -1 |
| G: -6289.08871 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.60455 HOMO: -6.69400 LUMO: -0.51974 factor:1 | 1 (-1.15014) | -1 | -1 |
| G: -6289.08871 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.38381 HOMO: -7.40422 LUMO: -0.98777 factor:1 | 1 (-0.92940) | -1 | -1 |
| G: -6289.08871 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.30209 HOMO: -6.88176 LUMO: -0.71022 factor:1 | 1 (-0.84769) | -1 | -1 |
| G: -6289.08871 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.56188 HOMO: -6.86271 LUMO: -0.59321 factor:1 | 1 (-1.10748) | -1 | -1 |
| G: -6289.08871 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.51208 HOMO: -6.73754 LUMO: -0.55239 factor:1 | 1 (-1.05768) | -1 | -1 |
| G: -6289.08871 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.11390 HOMO: -6.71033 LUMO: 1.57010 factor:1 | 1 (-0.65950) | -1 | -1 |
| G: -6289.08871 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.38879 HOMO: -6.69672 LUMO: 1.68711 factor:1 | 1 (-0.93438) | 1 | 1 |
| G: -6289.08871 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.31853 HOMO: -6.67495 LUMO: 2.03813 factor:1 | 1 (-0.86412) | 1 | 1 |
| G: -6289.08871 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.34990 HOMO: -6.54434 LUMO: 1.83677 factor:1 | 1 (-0.89550) | -1 | -1 |
| G: -6289.08871 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.18759 HOMO: -6.57155 LUMO: 1.77146 factor:1 | 1 (-0.73318) | 1 | 1 |
| G: -6289.08871 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.54659 HOMO: -6.76747 LUMO: 1.87759 factor:1 | 1 (-1.09218) | 1 | 1 |
| G: -6289.08871 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.32462 HOMO: -6.58243 LUMO: 1.61364 factor:1 | 1 (-0.87022) | 1 | 1 |
| G: -6289.08871 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.71787 HOMO: -6.61781 LUMO: 2.13881 factor:1 | 1 (-2.26347) | 1 | 1 |
| G: -6289.08871 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12556.50834 HOMO: -6.62597 LUMO: 2.00276 factor:1 | 1 (-3.05393) | 1 | 1 |
| G: -6289.08871 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12556.25900 HOMO: -7.01237 LUMO: 1.95922 factor:1 | 1 (-2.80460) | 1 | 1 |
| G: -6289.08871 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.60573 HOMO: -7.03959 LUMO: 2.16875 factor:1 | 1 (-2.15133) | 1 | 1 |
| G: -6289.08871 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.16707 HOMO: -6.83278 LUMO: 1.91296 factor:1 | 1 (-0.71267) | 1 | 1 |
| G: -6289.08871 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.39722 HOMO: -6.40012 LUMO: 1.95650 factor:1 | 1 (-0.94282) | -1 | -1 |
| G: -6289.08871 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.86778 HOMO: -6.50080 LUMO: 1.73337 factor:1 | 1 (-2.41338) | -1 | -1 |
| G: -6289.08871 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.19786 HOMO: -6.95795 LUMO: 2.28848 factor:1 | 1 (-1.74346) | 1 | 1 |
| G: -6289.08871 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12556.00384 HOMO: -6.63686 LUMO: 2.20140 factor:1 | 1 (-2.54943) | 1 | -1 |
| G: -6289.08871 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.90718 HOMO: -6.57427 LUMO: 1.87214 factor:1 | 1 (-2.45278) | 1 | -1 |
| G: -6289.08871 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.69028 HOMO: -6.38379 LUMO: 2.32113 factor:1 | 1 (-2.23588) | -1 | -1 |
| G: -6289.08871 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.97155 HOMO: -6.63958 LUMO: 2.04902 factor:1 | 1 (-1.51714) | 1 | 1 |
| G: -6289.08871 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.27920 HOMO: -6.70216 LUMO: 1.93201 factor:1 | 1 (-1.82480) | 1 | 1 |
| G: -6289.08871 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.40753 HOMO: -6.80557 LUMO: 2.23678 factor:1 | 1 (-1.95312) | 1 | 1 |
| G: -6289.08871 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.37204 HOMO: -6.72938 LUMO: 2.28304 factor:1 | 1 (-1.91764) | 1 | 1 |
| G: -6289.08871 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.35400 HOMO: -6.56067 LUMO: 1.66806 factor:1 | 1 (-1.89960) | -1 | -1 |
| G: -6289.08871 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.26965 HOMO: -6.95523 LUMO: 2.33474 factor:1 | 1 (-1.81524) | 1 | 1 |
| G: -6289.08871 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.56494 HOMO: -6.59876 LUMO: 2.30480 factor:1 | 1 (-2.11054) | 1 | 1 |
| G: -6289.08871 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.58816 HOMO: -6.87360 LUMO: 1.75786 factor:1 | 1 (-2.13375) | 1 | 1 |
| G: -6289.08871 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.36513 HOMO: -7.06408 LUMO: 1.99187 factor:1 | 1 (-1.91073) | 1 | 1 |
| G: -6289.08871 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.40862 HOMO: -6.95795 LUMO: 1.88847 factor:1 | 1 (-1.95421) | 1 | 1 |
| G: -6289.08871 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.10551 HOMO: -6.85455 LUMO: 1.63813 factor:1 | 1 (-1.65111) | 1 | 1 |
| G: -6289.08871 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.22761 HOMO: -7.09129 LUMO: 2.31569 factor:1 | 1 (-0.77321) | 1 | 1 |
| G: -6289.08871 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.08201 HOMO: -6.91441 LUMO: 1.68983 factor:1 | 1 (-0.62760) | 1 | 1 |
| G: -6289.08871 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.09991 HOMO: -6.89809 LUMO: 2.23678 factor:1 | 1 (-0.64551) | 1 | 1 |
| G: -6289.08871 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12553.83993 HOMO: -6.78652 LUMO: 1.98371 factor:1 | 1 (-0.38553) | 1 | -1 |
| G: -6289.08871 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.28459 HOMO: -6.94707 LUMO: 2.23678 factor:1 | 1 (-0.83019) | 1 | 1 |
| G: -6289.08871 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.99962 HOMO: -7.07224 LUMO: 2.13337 factor:1 | 1 (-2.54522) | 1 | 1 |
| G: -6289.08871 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.73978 HOMO: -6.94979 LUMO: 2.28031 factor:1 | 1 (-2.28538) | 1 | 1 |
| G: -6289.08871 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12556.05709 HOMO: -6.60965 LUMO: 2.20412 factor:1 | 1 (-2.60269) | 1 | 1 |
| G: -6289.08871 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.32848 HOMO: -6.87360 LUMO: 2.40277 factor:1 | 1 (-1.87408) | 1 | -1 |
| G: -6289.08871 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.05522 HOMO: -6.92802 LUMO: 1.89663 factor:1 | 1 (-1.60082) | 1 | -1 |
| G: -6289.08871 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.89976 HOMO: -6.88448 LUMO: 2.02725 factor:1 | 1 (-1.44536) | 1 | 1 |
| G: -6289.08871 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.09280 HOMO: -6.69128 LUMO: 1.55105 factor:1 | 1 (-1.63840) | -1 | -1 |
| G: -6289.08871 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.24516 HOMO: -6.54978 LUMO: 1.93201 factor:1 | 1 (-1.79075) | -1 | -1 |
| G: -6289.08871 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.22695 HOMO: -6.19331 LUMO: 1.46941 factor:1 | 1 (-1.77255) | -1 | -1 |
| G: -6289.08871 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.92885 HOMO: -6.55794 LUMO: 1.89663 factor:1 | 1 (-1.47445) | -1 | -1 |
| G: -6289.08871 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.04507 HOMO: -6.07630 LUMO: 1.94289 factor:1 | 1 (-1.59067) | -1 | -1 |
| G: -6289.08871 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.79405 HOMO: -7.46408 LUMO: 0.31565 factor:1 | 1 (-1.33964) | -1 | -1 |
| G: -6289.08871 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.23476 HOMO: -6.63958 LUMO: -0.61770 factor:1 | 1 (-1.78036) | -1 | -1 |
| G: -6289.08871 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.38944 HOMO: -6.81101 LUMO: -0.57960 factor:1 | 1 (-0.93504) | -1 | -1 |
| G: -6289.08871 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.58509 HOMO: -6.74298 LUMO: -0.57960 factor:1 | 1 (-1.13069) | -1 | -1 |
| G: -6289.08871 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.52014 HOMO: -6.63686 LUMO: -0.42994 factor:1 | 1 (-1.06573) | -1 | -1 |
| G: -6289.08871 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.48637 HOMO: -6.60965 LUMO: -0.41089 factor:1 | 1 (-1.03196) | -1 | -1 |
| G: -6289.08871 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.19240 HOMO: -6.60692 LUMO: -0.80274 factor:1 | 1 (-0.73800) | -1 | -1 |
| G: -6289.08871 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.33186 HOMO: -6.58788 LUMO: -0.78097 factor:1 | 1 (-0.87746) | -1 | -1 |
| G: -6289.08871 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.55497 HOMO: -6.67767 LUMO: -0.48436 factor:1 | 1 (-1.10056) | -1 | -1 |
| G: -6289.08871 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.78414 HOMO: -6.63141 LUMO: -0.40545 factor:1 | 1 (-1.32974) | -1 | -1 |
| G: -6289.08871 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.75535 HOMO: -6.62053 LUMO: -0.83811 factor:1 | 1 (-1.30095) | -1 | -1 |
| G: -6289.08871 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.48022 HOMO: -6.59604 LUMO: -0.35375 factor:1 | 1 (-1.02581) | -1 | -1 |
| G: -6289.08871 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.55739 HOMO: -6.34297 LUMO: -0.39729 factor:1 | 1 (-1.10299) | -1 | -1 |
| G: -6289.08871 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.23123 HOMO: -6.67223 LUMO: 1.97827 factor:1 | 1 (-0.77683) | 1 | 1 |
| G: -6289.08871 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.33513 HOMO: -6.40012 LUMO: 1.89935 factor:1 | 1 (-0.88072) | -1 | -1 |
| G: -6289.08871 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.20522 HOMO: -6.74842 LUMO: 1.97283 factor:1 | 1 (-0.75082) | 1 | -1 |
| G: -6289.08871 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.04503 HOMO: -6.76747 LUMO: 2.17147 factor:1 | 1 (-0.59062) | 1 | 1 |
| G: -6289.08871 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.33567 HOMO: -6.72121 LUMO: 1.55649 factor:1 | 1 (-0.88127) | -1 | -1 |
| G: -6289.08871 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.57415 HOMO: -6.97700 LUMO: 2.04085 factor:1 | 1 (-1.11975) | 1 | 1 |
| G: -6289.08871 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.62776 HOMO: -7.06680 LUMO: 2.04085 factor:1 | 1 (-1.17335) | 1 | -1 |
| G: -6289.08871 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.35330 HOMO: -7.09673 LUMO: 2.35106 factor:1 | 1 (-0.89890) | 1 | 1 |
| G: -6289.08871 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.57284 HOMO: -6.83006 LUMO: 2.14970 factor:1 | 1 (-1.11844) | 1 | 1 |
| G: -6289.08871 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.47042 HOMO: -6.72665 LUMO: 2.20140 factor:1 | 1 (-1.01602) | 1 | -1 |
| G: -6289.08871 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.67026 HOMO: -6.77291 LUMO: 2.34562 factor:1 | 1 (-1.21586) | 1 | -1 |
| G: -6289.08871 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.17052 HOMO: -6.73754 LUMO: 2.00276 factor:1 | 1 (-1.71611) | 1 | -1 |
| G: -6289.08871 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.33591 HOMO: -7.04231 LUMO: 1.92112 factor:1 | 1 (-1.88150) | 1 | -1 |
| G: -6289.08871 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.04330 HOMO: -6.83822 LUMO: 1.72248 factor:1 | 1 (-1.58890) | 1 | 1 |
| G: -6289.08871 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.11054 HOMO: -6.57971 LUMO: 2.16603 factor:1 | 1 (-1.65614) | 1 | -1 |
| G: -6289.08871 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.02442 HOMO: -6.80013 LUMO: 1.88575 factor:1 | 1 (-1.57002) | 1 | 1 |
| G: -6289.08871 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.08181 HOMO: -6.93618 LUMO: 2.18235 factor:1 | 1 (-1.62740) | 1 | 1 |
| G: -6289.08871 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.56985 HOMO: -6.54706 LUMO: 1.91024 factor:1 | 1 (-1.11545) | -1 | -1 |
| G: -6289.08871 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.31379 HOMO: -7.06952 LUMO: 2.18507 factor:1 | 1 (-0.85939) | 1 | 1 |
| G: -6289.08871 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.13295 HOMO: -7.05047 LUMO: 1.82044 factor:1 | 1 (-0.67854) | 1 | 1 |
| G: -6289.08871 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12553.95498 HOMO: -6.87632 LUMO: 1.92657 factor:1 | 1 (-0.50058) | 1 | 1 |
| G: -6289.08871 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.25401 HOMO: -6.58788 LUMO: 1.91568 factor:1 | 1 (-0.79961) | 1 | -1 |
| G: -6289.08871 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.38432 HOMO: -7.17292 LUMO: 1.90752 factor:1 | 1 (-0.92992) | 1 | 1 |
| G: -6289.08871 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.34198 HOMO: -6.93890 LUMO: 1.80684 factor:1 | 1 (-0.88758) | 1 | 1 |
| G: -6289.08871 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.29774 HOMO: -7.10761 LUMO: 2.20956 factor:1 | 1 (-0.84334) | 1 | 1 |
| G: -6289.08871 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.05771 HOMO: -6.85727 LUMO: 2.13609 factor:1 | 1 (-0.60330) | 1 | -1 |
| G: -6289.08871 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.25414 HOMO: -6.64502 LUMO: 1.38506 factor:1 | 1 (-0.79974) | -1 | -1 |
| G: -6289.08871 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.15757 HOMO: -6.87360 LUMO: 1.15648 factor:1 | 1 (-0.70317) | -1 | -1 |
| G: -6289.08871 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12553.84864 HOMO: -6.67223 LUMO: 2.07351 factor:1 | 1 (-0.39424) | 1 | 1 |
| G: -6289.08871 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.50375 HOMO: -6.29671 LUMO: 2.43270 factor:1 | 1 (-1.04935) | -1 | -1 |
| G: -6289.08871 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.16968 HOMO: -6.90897 LUMO: 2.28848 factor:1 | 1 (-0.71528) | 1 | 1 |
| G: -6289.08871 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.49959 HOMO: -7.04231 LUMO: 1.70071 factor:1 | 1 (-1.04519) | 1 | 1 |
| G: -6289.08871 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.33608 HOMO: -6.69944 LUMO: 1.94834 factor:1 | 1 (-0.88168) | 1 | 1 |
| G: -6289.08871 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.13009 HOMO: -6.56067 LUMO: 2.20956 factor:1 | 1 (-0.67569) | -1 | -1 |
| G: -6289.08871 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12553.82959 HOMO: -6.65046 LUMO: 2.06807 factor:1 | 1 (-0.37519) | 1 | -1 |
| G: -6289.08871 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.32528 HOMO: -7.08584 LUMO: 1.98915 factor:1 | 1 (-0.87087) | 1 | 1 |
| G: -6289.08871 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.51233 HOMO: -6.69400 LUMO: 2.09256 factor:1 | 1 (-1.05792) | 1 | 1 |
| G: -6289.08871 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.45235 HOMO: -6.62869 LUMO: 2.16331 factor:1 | 1 (-0.99795) | 1 | 1 |
| G: -6289.08871 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.26253 HOMO: -6.85183 LUMO: 2.16058 factor:1 | 1 (-0.80812) | 1 | 1 |
| G: -6289.08871 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.26508 HOMO: -6.54706 LUMO: 1.92384 factor:1 | 1 (-0.81068) | -1 | -1 |
| G: -6289.08871 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12553.90959 HOMO: -6.84366 LUMO: 2.48984 factor:1 | 1 (-0.45519) | 1 | 1 |
| G: -6289.08871 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.08103 HOMO: -6.77291 LUMO: 2.46263 factor:1 | 1 (-0.62662) | 1 | 1 |
| G: -6289.08871 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.10432 HOMO: -7.01782 LUMO: 2.31025 factor:1 | 1 (-0.64992) | 1 | 1 |
| G: -6289.08871 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12553.83237 HOMO: -6.94707 LUMO: 2.29664 factor:1 | 1 (-0.37797) | 1 | 1 |
| G: -6289.08871 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.36974 HOMO: -6.64230 LUMO: 1.97283 factor:1 | 1 (-0.91534) | 1 | 1 |
| G: -6289.08871 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.66830 HOMO: -6.47359 LUMO: 2.20412 factor:1 | 1 (-1.21390) | -1 | -1 |
| G: -6289.08871 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.43494 HOMO: -6.90625 LUMO: 1.92384 factor:1 | 1 (-0.98054) | 1 | 1 |
| G: -6289.08871 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.58071 HOMO: -7.17020 LUMO: 2.06807 factor:1 | 1 (-1.12631) | 1 | 1 |
| G: -6289.08871 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.66626 HOMO: -6.65046 LUMO: 2.20956 factor:1 | 1 (-1.21186) | 1 | -1 |
| G: -6289.08871 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.72863 HOMO: -7.07496 LUMO: 1.82861 factor:1 | 1 (-1.27423) | 1 | 1 |
| G: -6289.08871 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.43926 HOMO: -6.83006 LUMO: 2.14970 factor:1 | 1 (-0.98486) | 1 | -1 |
| G: -6289.08871 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.39200 HOMO: -6.92802 LUMO: 1.99187 factor:1 | 1 (-0.93760) | 1 | 1 |
| G: -6289.08871 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.64134 HOMO: -6.69672 LUMO: 2.36739 factor:1 | 1 (-1.18693) | 1 | -1 |
| G: -6289.08871 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.34030 HOMO: -7.13755 LUMO: 2.00276 factor:1 | 1 (-0.88589) | 1 | 1 |
| G: -6289.08871 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.58479 HOMO: -6.92530 LUMO: 2.25582 factor:1 | 1 (-1.13039) | 1 | 1 |
| G: -6289.08871 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.62939 HOMO: -6.77564 LUMO: 1.97827 factor:1 | 1 (-1.17499) | 1 | 1 |
| G: -6289.08871 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.41983 HOMO: -6.87904 LUMO: 1.60003 factor:1 | 1 (-0.96543) | 1 | 1 |
| G: -6289.08871 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.28323 HOMO: -6.62869 LUMO: 1.90480 factor:1 | 1 (-0.82883) | 1 | 1 |
| G: -6289.08871 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.36514 HOMO: -6.71033 LUMO: 1.54833 factor:1 | 1 (-0.91074) | -1 | -1 |
| G: -6289.08871 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.48258 HOMO: -6.74298 LUMO: 1.47486 factor:1 | 1 (-1.02818) | -1 | -1 |
| G: -6289.08871 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.52792 HOMO: -6.77019 LUMO: 1.90480 factor:1 | 1 (-1.07352) | 1 | 1 |
| G: -6289.08871 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.32729 HOMO: -6.70489 LUMO: 1.99459 factor:1 | 1 (-0.87289) | 1 | 1 |
| G: -6289.08871 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.14002 HOMO: -6.73482 LUMO: 2.08711 factor:1 | 1 (-0.68562) | 1 | 1 |
| G: -6289.08871 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12553.86426 HOMO: -6.46543 LUMO: 1.73881 factor:1 | 1 (-0.40986) | -1 | -1 |
| G: -6289.08871 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.39219 HOMO: -6.96067 LUMO: 2.26127 factor:1 | 1 (-0.93779) | 1 | 1 |
| G: -6289.08871 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.37025 HOMO: -6.67767 LUMO: 2.10616 factor:1 | 1 (-1.91584) | 1 | 1 |
| G: -6289.08871 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.39411 HOMO: -6.28855 LUMO: 2.35923 factor:1 | 1 (-1.93971) | -1 | -1 |
| G: -6289.08871 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.37863 HOMO: -6.80285 LUMO: 1.62724 factor:1 | 1 (-1.92423) | 1 | 1 |
| G: -6289.08871 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.95620 HOMO: -6.85455 LUMO: 2.23133 factor:1 | 1 (-1.50180) | 1 | 1 |
| G: -6289.08871 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.18173 HOMO: -6.51713 LUMO: 2.33474 factor:1 | 1 (-1.72732) | -1 | -1 |
| G: -6289.08871 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.09231 HOMO: -6.88176 LUMO: 2.15242 factor:1 | 1 (-1.63791) | 1 | 1 |
| G: -6289.08871 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.16377 HOMO: -6.54434 LUMO: 2.32113 factor:1 | 1 (-1.70936) | -1 | -1 |
| G: -6289.08871 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.60196 HOMO: -6.62597 LUMO: 2.24222 factor:1 | 1 (-1.14756) | 1 | 1 |
| G: -6289.08871 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.35189 HOMO: -6.74570 LUMO: 2.19868 factor:1 | 1 (-0.89749) | 1 | 1 |
| G: -6289.08871 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.38612 HOMO: -6.62869 LUMO: 1.98915 factor:1 | 1 (-0.93172) | 1 | 1 |
| G: -6289.08871 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.20595 HOMO: -6.64502 LUMO: 2.13881 factor:1 | 1 (-0.75155) | 1 | 1 |
| G: -6289.08871 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.16097 HOMO: -6.95795 LUMO: 1.82316 factor:1 | 1 (-0.70657) | 1 | 1 |
| G: -6289.08871 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.10116 HOMO: -6.77291 LUMO: 1.36329 factor:1 | 1 (-0.64676) | -1 | -1 |
| G: -6289.08871 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12553.93531 HOMO: -6.45726 LUMO: 1.73064 factor:1 | 1 (-0.48091) | -1 | -1 |
| G: -6289.08871 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.35110 HOMO: -6.49264 LUMO: 1.77418 factor:1 | 1 (-0.89670) | -1 | -1 |
| G: -6289.08871 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.32440 HOMO: -6.60420 LUMO: 2.20956 factor:1 | 1 (-0.87000) | 1 | 1 |
| G: -6289.08871 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.20744 HOMO: -6.56067 LUMO: 2.05718 factor:1 | 1 (-1.75304) | -1 | -1 |
| G: -6289.08871 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.05487 HOMO: -6.62597 LUMO: 1.70343 factor:1 | 1 (-1.60046) | 1 | 1 |
| G: -6289.08871 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.49463 HOMO: -6.69400 LUMO: 2.16875 factor:1 | 1 (-2.04023) | 1 | 1 |
| G: -6289.08871 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.84360 HOMO: -6.63958 LUMO: 2.11977 factor:1 | 1 (-1.38920) | 1 | 1 |
| G: -6289.08871 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.88308 HOMO: -6.92802 LUMO: 1.82044 factor:1 | 1 (-1.42868) | 1 | -1 |
| G: -6289.08871 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.97971 HOMO: -6.56339 LUMO: 2.30480 factor:1 | 1 (-1.52531) | -1 | -1 |
| G: -6289.08871 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.00752 HOMO: -6.63958 LUMO: 1.91024 factor:1 | 1 (-1.55312) | 1 | -1 |
| G: -6289.08871 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.14012 HOMO: -6.93074 LUMO: 2.05446 factor:1 | 1 (-1.68572) | 1 | 1 |
| G: -6289.08871 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.13383 HOMO: -6.61509 LUMO: 2.03813 factor:1 | 1 (-1.67943) | 1 | 1 |
| G: -6289.08871 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.04123 HOMO: -6.61237 LUMO: 1.91296 factor:1 | 1 (-1.58683) | 1 | -1 |
| G: -6289.08871 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.98518 HOMO: -6.86815 LUMO: 1.95378 factor:1 | 1 (-1.53078) | 1 | 1 |
| G: -6289.08871 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.75995 HOMO: -6.63686 LUMO: 1.70888 factor:1 | 1 (-1.30555) | 1 | 1 |
| G: -6289.08871 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.87633 HOMO: -6.57971 LUMO: 2.20140 factor:1 | 1 (-1.42193) | 1 | -1 |
| G: -6289.08871 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.93152 HOMO: -6.41100 LUMO: 1.96738 factor:1 | 1 (-1.47712) | -1 | -1 |
| G: -6289.08871 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.22355 HOMO: -6.90081 LUMO: 1.65989 factor:1 | 1 (-1.76915) | 1 | 1 |
| G: -6289.08871 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.00306 HOMO: -6.68312 LUMO: 1.97827 factor:1 | 1 (-1.54865) | 1 | -1 |
| G: -6289.08871 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.05166 HOMO: -6.65318 LUMO: 2.10888 factor:1 | 1 (-1.59725) | 1 | -1 |
| G: -6289.08871 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.29898 HOMO: -6.62053 LUMO: 2.28848 factor:1 | 1 (-1.84458) | 1 | -1 |
| G: -6289.08871 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12556.42110 HOMO: -6.65863 LUMO: 2.29664 factor:1 | 1 (-2.96669) | 1 | -1 |
| G: -6289.08871 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.79624 HOMO: -6.63958 LUMO: 2.07623 factor:1 | 1 (-2.34184) | 1 | -1 |
| G: -6289.08871 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12556.57737 HOMO: -6.58243 LUMO: 2.20684 factor:1 | 1 (-3.12297) | 1 | 1 |
| G: -6289.08871 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.59235 HOMO: -6.59332 LUMO: 2.05174 factor:1 | 1 (-2.13794) | 1 | -1 |
| G: -6289.08871 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.61006 HOMO: -6.95251 LUMO: 2.20140 factor:1 | 1 (-2.15566) | 1 | 1 |
| G: -6289.08871 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12556.43644 HOMO: -6.84638 LUMO: 2.39732 factor:1 | 1 (-2.98204) | 1 | 1 |
| G: -6289.08871 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12556.39827 HOMO: -6.86815 LUMO: 2.47896 factor:1 | 1 (-2.94386) | 1 | 1 |
| G: -6289.08871 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12556.01633 HOMO: -7.00693 LUMO: 2.43270 factor:1 | 1 (-2.56192) | 1 | 1 |
| G: -6289.08871 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12556.39759 HOMO: -6.58788 LUMO: 2.30208 factor:1 | 1 (-2.94318) | 1 | 1 |
| G: -6289.08871 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12556.20077 HOMO: -6.63958 LUMO: 2.28031 factor:1 | 1 (-2.74636) | 1 | 1 |
| G: -6289.08871 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.41242 HOMO: -6.74570 LUMO: 2.28304 factor:1 | 1 (-1.95802) | 1 | 1 |
| G: -6289.08871 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.98346 HOMO: -6.78380 LUMO: 2.16331 factor:1 | 1 (-1.52906) | 1 | 1 |
| G: -6289.08871 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12556.16076 HOMO: -6.52529 LUMO: 2.05718 factor:1 | 1 (-2.70636) | -1 | -1 |
| G: -6289.08871 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.26867 HOMO: -6.41644 LUMO: 1.65445 factor:1 | 1 (-1.81426) | -1 | -1 |
| G: -6289.08871 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.42004 HOMO: -6.34570 LUMO: 1.22451 factor:1 | 1 (-1.96564) | -1 | -1 |
| G: -6289.08871 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.04847 HOMO: -6.14433 LUMO: 1.85582 factor:1 | 1 (-1.59407) | -1 | -1 |
| G: -6289.08871 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.61213 HOMO: -6.62053 LUMO: 1.92112 factor:1 | 1 (-2.15773) | 1 | -1 |
| G: -6289.08871 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.33278 HOMO: -6.63414 LUMO: 1.61908 factor:1 | 1 (-1.87837) | 1 | 1 |
| G: -6289.08871 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.43545 HOMO: -6.75931 LUMO: 1.87214 factor:1 | 1 (-1.98104) | 1 | 1 |
| G: -6289.08871 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.48143 HOMO: -6.55794 LUMO: 1.77418 factor:1 | 1 (-2.02703) | -1 | -1 |
| G: -6289.08871 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.35574 HOMO: -6.52801 LUMO: 1.82044 factor:1 | 1 (-1.90134) | -1 | -1 |
| G: -6289.08871 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.79926 HOMO: -6.77564 LUMO: 1.97827 factor:1 | 1 (-2.34486) | 1 | 1 |
| G: -6289.08871 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.60688 HOMO: -6.93890 LUMO: 1.81228 factor:1 | 1 (-2.15248) | 1 | 1 |
| G: -6289.08871 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.64473 HOMO: -6.85455 LUMO: 1.75513 factor:1 | 1 (-2.19033) | 1 | 1 |
| G: -6289.08871 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.61575 HOMO: -6.86815 LUMO: 1.64629 factor:1 | 1 (-2.16135) | 1 | 1 |
| G: -6289.08871 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.23956 HOMO: -6.98516 LUMO: 1.84765 factor:1 | 1 (-0.78516) | 1 | 1 |
| G: -6289.08871 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.40013 HOMO: -6.04637 LUMO: 1.94017 factor:1 | 1 (-0.94573) | -1 | -1 |
| G: -6289.08871 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.24974 HOMO: -6.86271 LUMO: 2.11977 factor:1 | 1 (-0.79533) | 1 | -1 |
| G: -6289.08871 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.44525 HOMO: -6.72938 LUMO: 2.11160 factor:1 | 1 (-0.99085) | 1 | -1 |
| G: -6289.08871 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.32143 HOMO: -7.01782 LUMO: 2.13609 factor:1 | 1 (-1.86703) | 1 | 1 |
| G: -6289.08871 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12556.03823 HOMO: -6.18515 LUMO: 2.04630 factor:1 | 1 (-2.58383) | -1 | -1 |
| G: -6289.08871 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.97173 HOMO: -6.60965 LUMO: 2.17147 factor:1 | 1 (-2.51733) | 1 | -1 |
| G: -6289.08871 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.33612 HOMO: -6.87360 LUMO: 2.35378 factor:1 | 1 (-1.88172) | 1 | 1 |
| G: -6289.08871 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.81398 HOMO: -6.72938 LUMO: 2.20140 factor:1 | 1 (-2.35958) | 1 | -1 |
| G: -6289.08871 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.16886 HOMO: -6.88448 LUMO: 2.54154 factor:1 | 1 (-1.71445) | 1 | -1 |
| G: -6289.08871 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.36393 HOMO: -6.87087 LUMO: 2.16058 factor:1 | 1 (-1.90953) | 1 | 1 |
| G: -6289.08871 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.28576 HOMO: -7.11306 LUMO: 2.04085 factor:1 | 1 (-1.83135) | 1 | 1 |
| G: -6289.08871 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.25599 HOMO: -6.66951 LUMO: 1.68438 factor:1 | 1 (-1.80158) | 1 | 1 |
| G: -6289.08871 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.29974 HOMO: -7.08312 LUMO: 2.19324 factor:1 | 1 (-1.84534) | 1 | 1 |
| G: -6289.08871 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.93582 HOMO: -6.69128 LUMO: 2.13881 factor:1 | 1 (-1.48142) | 1 | -1 |
| G: -6289.08871 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.07421 HOMO: -6.80285 LUMO: 2.16603 factor:1 | 1 (-1.61981) | 1 | 1 |
| G: -6289.08871 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.04017 HOMO: -6.82189 LUMO: 2.46807 factor:1 | 1 (-1.58577) | 1 | 1 |
| G: -6289.08871 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.86632 HOMO: -6.78652 LUMO: 2.12521 factor:1 | 1 (-1.41192) | 1 | 1 |
| G: -6289.08871 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.26083 HOMO: -6.47903 LUMO: 1.70071 factor:1 | 1 (-1.80643) | -1 | -1 |
| G: -6289.08871 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.38555 HOMO: -6.37019 LUMO: 1.24356 factor:1 | 1 (-0.93115) | -1 | -1 |
| G: -6289.08871 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.45328 HOMO: -6.69400 LUMO: 1.67350 factor:1 | 1 (-0.99888) | 1 | 1 |
| G: -6289.08871 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.25058 HOMO: -7.51851 LUMO: 0.27756 factor:1 | 1 (-0.79618) | -1 | -1 |
| G: -6289.08871 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.45698 HOMO: -6.95795 LUMO: -0.72110 factor:1 | 1 (-1.00258) | -1 | -1 |
| G: -6289.08871 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.30566 HOMO: -6.88720 LUMO: -0.67484 factor:1 | 1 (-0.85125) | -1 | -1 |
| G: -6289.08871 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.44824 HOMO: -6.83550 LUMO: -0.57144 factor:1 | 1 (-0.99384) | -1 | -1 |
| G: -6289.08871 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.22242 HOMO: -6.80285 LUMO: -0.57144 factor:1 | 1 (-0.76801) | -1 | -1 |
| G: -6289.08871 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.42819 HOMO: -6.76475 LUMO: -0.53062 factor:1 | 1 (-0.97379) | -1 | -1 |
| G: -6289.08871 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.32177 HOMO: -6.66951 LUMO: 1.74969 factor:1 | 1 (-0.86736) | 1 | 1 |
| G: -6289.08871 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.26503 HOMO: -6.53345 LUMO: 1.89935 factor:1 | 1 (-0.81063) | -1 | -1 |
| G: -6289.08871 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.46318 HOMO: -6.65046 LUMO: 2.01364 factor:1 | 1 (-1.00878) | 1 | -1 |
| G: -6289.08871 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.29115 HOMO: -6.64230 LUMO: 2.11977 factor:1 | 1 (-0.83675) | 1 | -1 |
| G: -6289.08871 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.26315 HOMO: -6.44910 LUMO: 2.13337 factor:1 | 1 (-0.80875) | -1 | -1 |
| G: -6289.08871 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.31172 HOMO: -7.05591 LUMO: 1.98915 factor:1 | 1 (-0.85732) | 1 | -1 |
| G: -6289.08871 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.23423 HOMO: -7.02326 LUMO: 2.49256 factor:1 | 1 (-0.77982) | 1 | 1 |
| G: -6289.08871 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.36865 HOMO: -6.32937 LUMO: 2.51161 factor:1 | 1 (-0.91425) | -1 | -1 |
| G: -6289.08871 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.31276 HOMO: -6.96067 LUMO: 2.20140 factor:1 | 1 (-0.85836) | 1 | 1 |
| G: -6289.08871 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.51565 HOMO: -6.97972 LUMO: 2.55243 factor:1 | 1 (-1.06124) | 1 | 1 |
| G: -6289.08871 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.41026 HOMO: -6.72665 LUMO: 2.46535 factor:1 | 1 (-0.95585) | 1 | 1 |
| G: -6289.08871 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.28922 HOMO: -6.41917 LUMO: 2.35106 factor:1 | 1 (-0.83482) | -1 | -1 |
| G: -6289.08871 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12553.97528 HOMO: -6.75114 LUMO: 2.32929 factor:1 | 1 (-0.52088) | 1 | 1 |
| G: -6289.08871 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.20859 HOMO: -6.91713 LUMO: 2.27215 factor:1 | 1 (-0.75419) | 1 | 1 |
| G: -6289.08871 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.40326 HOMO: -6.54978 LUMO: 2.00276 factor:1 | 1 (-0.94886) | -1 | -1 |
| G: -6289.08871 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.19643 HOMO: -6.62325 LUMO: 2.05990 factor:1 | 1 (-0.74203) | 1 | 1 |
| G: -6289.08871 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.41047 HOMO: -6.86271 LUMO: 2.14970 factor:1 | 1 (-0.95607) | 1 | 1 |
| G: -6289.08871 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.32620 HOMO: -6.77564 LUMO: 2.25855 factor:1 | 1 (-0.87180) | 1 | -1 |
| G: -6289.08871 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.23409 HOMO: -6.71305 LUMO: 1.94561 factor:1 | 1 (-0.77969) | 1 | -1 |
| G: -6289.08871 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.43760 HOMO: -6.75659 LUMO: 1.94561 factor:1 | 1 (-0.98320) | 1 | -1 |
| G: -6289.08871 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.50642 HOMO: -6.94979 LUMO: 2.33474 factor:1 | 1 (-1.05202) | 1 | -1 |
| G: -6289.08871 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.96665 HOMO: -6.85727 LUMO: 2.50345 factor:1 | 1 (-1.51225) | 1 | -1 |
| G: -6289.08871 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.04978 HOMO: -6.87360 LUMO: 2.43270 factor:1 | 1 (-1.59538) | 1 | -1 |
| G: -6289.08871 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.90112 HOMO: -6.57427 LUMO: 2.46807 factor:1 | 1 (-1.44672) | 1 | -1 |
| G: -6289.08871 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.00159 HOMO: -7.16204 LUMO: 2.15242 factor:1 | 1 (-1.54718) | 1 | 1 |
| G: -6289.08871 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.08730 HOMO: -6.62869 LUMO: 2.11432 factor:1 | 1 (-1.63290) | 1 | -1 |
| G: -6289.08871 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.22344 HOMO: -7.05591 LUMO: 2.26671 factor:1 | 1 (-1.76904) | 1 | -1 |
| G: -6289.08871 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.36336 HOMO: -7.13483 LUMO: 1.47758 factor:1 | 1 (-1.90896) | -1 | -1 |
| G: -6289.08871 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.96719 HOMO: -6.72938 LUMO: 1.57282 factor:1 | 1 (-1.51279) | -1 | -1 |
| G: -6289.08871 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.45822 HOMO: -6.17426 LUMO: 1.81228 factor:1 | 1 (-2.00382) | -1 | -1 |
| G: -6289.08871 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12556.38678 HOMO: -6.65318 LUMO: 1.93473 factor:1 | 1 (-2.93238) | 1 | -1 |
| G: -6289.08871 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12556.16795 HOMO: -6.18515 LUMO: 2.01364 factor:1 | 1 (-2.71355) | -1 | -1 |
| G: -6289.08871 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12556.42335 HOMO: -7.05591 LUMO: 2.13337 factor:1 | 1 (-2.96895) | 1 | 1 |
| G: -6289.08871 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.50184 HOMO: -6.90897 LUMO: 2.29664 factor:1 | 1 (-2.04744) | 1 | -1 |
| G: -6289.08871 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12556.01902 HOMO: -7.11034 LUMO: 2.17147 factor:1 | 1 (-2.56462) | 1 | 1 |
| G: -6289.08871 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.41030 HOMO: -6.82734 LUMO: 2.26671 factor:1 | 1 (-1.95590) | 1 | 1 |
| G: -6289.08871 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12556.20528 HOMO: -6.34842 LUMO: 2.34562 factor:1 | 1 (-2.75088) | -1 | -1 |
| G: -6289.08871 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12556.26485 HOMO: -6.62053 LUMO: 2.22861 factor:1 | 1 (-2.81045) | 1 | -1 |
| G: -6289.08871 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.24129 HOMO: -6.80557 LUMO: 2.07079 factor:1 | 1 (-1.78689) | 1 | -1 |
| G: -6289.08871 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12556.05448 HOMO: -6.60692 LUMO: 2.46263 factor:1 | 1 (-2.60008) | 1 | -1 |
| G: -6289.08871 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.45700 HOMO: -7.02054 LUMO: 2.08711 factor:1 | 1 (-2.00259) | 1 | -1 |
| G: -6289.08871 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.27988 HOMO: -6.78652 LUMO: 2.02453 factor:1 | 1 (-1.82548) | 1 | 1 |
| G: -6289.08871 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.18823 HOMO: -6.51168 LUMO: 2.06534 factor:1 | 1 (-1.73383) | -1 | -1 |
| G: -6289.08871 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.34099 HOMO: -6.50080 LUMO: 2.01636 factor:1 | 1 (-1.88659) | -1 | -1 |
| G: -6289.08871 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.40932 HOMO: -6.54434 LUMO: 1.84493 factor:1 | 1 (-1.95492) | -1 | -1 |
| G: -6289.08871 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.26045 HOMO: -6.47087 LUMO: 1.76330 factor:1 | 1 (-1.80605) | -1 | -1 |
| G: -6289.08871 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.96940 HOMO: -6.78924 LUMO: 2.39460 factor:1 | 1 (-1.51499) | 1 | 1 |
| G: -6289.08871 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.46758 HOMO: -6.59876 LUMO: 1.84493 factor:1 | 1 (-2.01318) | 1 | 1 |
| G: -6289.08871 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.38114 HOMO: -6.41644 LUMO: 2.05174 factor:1 | 1 (-0.92674) | -1 | -1 |
| G: -6289.08871 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.39728 HOMO: -6.52257 LUMO: 2.11160 factor:1 | 1 (-0.94287) | -1 | -1 |
| G: -6289.08871 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.35328 HOMO: -6.90897 LUMO: 2.34018 factor:1 | 1 (-0.89887) | 1 | 1 |
| G: -6289.08871 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12553.98236 HOMO: -6.97428 LUMO: 1.86126 factor:1 | 1 (-0.52796) | 1 | 1 |
| G: -6289.08871 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.16582 HOMO: -7.13483 LUMO: 2.14698 factor:1 | 1 (-0.71141) | 1 | -1 |
| G: -6289.08871 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.25055 HOMO: -7.16748 LUMO: 2.31841 factor:1 | 1 (-0.79615) | 1 | 1 |
| G: -6289.08871 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12553.91675 HOMO: -6.87087 LUMO: 2.38916 factor:1 | 1 (-0.46235) | 1 | -1 |
| G: -6289.08871 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.11776 HOMO: -6.93074 LUMO: 2.42181 factor:1 | 1 (-0.66336) | 1 | -1 |
| G: -6289.08871 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.27458 HOMO: -6.90081 LUMO: 2.00276 factor:1 | 1 (-0.82018) | 1 | -1 |
| G: -6289.08871 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.17681 HOMO: -6.99333 LUMO: 2.03541 factor:1 | 1 (-0.72241) | 1 | 1 |
| G: -6289.08871 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.62326 HOMO: -6.89264 LUMO: 1.57554 factor:1 | 1 (-2.16886) | -1 | -1 |
| G: -6289.08871 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.35580 HOMO: -6.48175 LUMO: 1.85854 factor:1 | 1 (-1.90140) | -1 | -1 |
| G: -6289.08871 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12556.39514 HOMO: -6.69400 LUMO: 1.62452 factor:1 | 1 (-2.94073) | 1 | 1 |
| G: -6289.08871 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12556.30681 HOMO: -6.50896 LUMO: 1.88303 factor:1 | 1 (-2.85241) | -1 | -1 |
| G: -6289.08871 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12556.17853 HOMO: -6.60420 LUMO: 2.05990 factor:1 | 1 (-2.72413) | 1 | 1 |
| G: -6289.08871 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.19373 HOMO: -7.14299 LUMO: 2.07351 factor:1 | 1 (-1.73932) | 1 | 1 |
| G: -6289.08871 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12553.87792 HOMO: -7.06408 LUMO: 1.81228 factor:1 | 1 (-0.42352) | 1 | 1 |
| G: -6289.08871 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.09156 HOMO: -6.67495 LUMO: 1.79595 factor:1 | 1 (-0.63715) | 1 | 1 |
| G: -6289.08871 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.24691 HOMO: -6.45182 LUMO: 2.15786 factor:1 | 1 (-0.79250) | -1 | -1 |
| G: -6289.08871 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.83445 HOMO: -6.93346 LUMO: 2.45719 factor:1 | 1 (-2.38004) | 1 | 1 |
| G: -6289.08871 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.80266 HOMO: -6.50080 LUMO: 2.08167 factor:1 | 1 (-2.34826) | -1 | -1 |
| G: -6289.08871 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.00401 HOMO: -6.83550 LUMO: -0.67484 factor:1 | 1 (-1.54961) | -1 | -1 |
| G: -6289.08871 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.69183 HOMO: -7.04231 LUMO: 0.54151 factor:1 | 1 (-2.23743) | -1 | -1 |
| G: -6289.08871 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.87652 HOMO: -6.79740 LUMO: 1.91296 factor:1 | 1 (-1.42212) | -1 | -1 |
| G: -6289.08871 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.90262 HOMO: -7.35796 LUMO: -1.04220 factor:1 | 1 (-1.44822) | -1 | -1 |
| G: -6289.08871 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.88136 HOMO: -6.62597 LUMO: -0.44082 factor:1 | 1 (-2.42696) | -1 | -1 |
| G: -6289.08871 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.09870 HOMO: -6.45182 LUMO: -0.20409 factor:1 | 1 (-1.64430) | -1 | -1 |
| G: -6289.08871 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.11990 HOMO: -6.51168 LUMO: -0.23130 factor:1 | 1 (-1.66550) | -1 | -1 |
| G: -6289.08871 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.23016 HOMO: -7.14027 LUMO: 0.49797 factor:1 | 1 (-1.77576) | -1 | -1 |
| G: -6289.33611 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.24925 HOMO: -7.55660 LUMO: 0.24762 factor:1 | 1 (-0.54744) | -1 | -1 |
| G: -6289.33611 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.74863 HOMO: -6.88992 LUMO: -0.64763 factor:1 | 1 (-1.04682) | -1 | -1 |
| G: -6289.33611 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12556.64135 HOMO: -6.72665 LUMO: -0.45987 factor:1 | 1 (-2.93954) | -1 | -1 |
| G: -6289.33611 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12556.08155 HOMO: -6.72121 LUMO: -0.58232 factor:1 | 1 (-2.37974) | -1 | -1 |
| G: -6289.33611 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.70810 HOMO: -7.26816 LUMO: 0.32926 factor:1 | 1 (-2.00630) | -1 | -1 |
| G: -6289.33611 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.66202 HOMO: -6.57155 LUMO: -0.53606 factor:1 | 1 (-0.96021) | -1 | -1 |
| G: -6289.33611 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.40056 HOMO: -6.50896 LUMO: -0.43810 factor:1 | 1 (-1.69875) | -1 | -1 |
| G: -6289.33611 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.48611 HOMO: -6.73210 LUMO: -0.51430 factor:1 | 1 (-1.78431) | -1 | -1 |
| G: -6289.33611 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12556.10906 HOMO: -6.77019 LUMO: -0.62858 factor:1 | 1 (-2.40726) | -1 | -1 |
| G: -6289.33611 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.41662 HOMO: -6.82462 LUMO: -0.67484 factor:1 | 1 (-1.71481) | -1 | -1 |
| G: -6289.33611 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.97246 HOMO: -6.79740 LUMO: -0.55511 factor:1 | 1 (-2.27065) | -1 | -1 |
| G: -6289.33611 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12556.00275 HOMO: -6.79740 LUMO: -0.67756 factor:1 | 1 (-2.30094) | -1 | -1 |
| G: -6289.33611 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.69451 HOMO: -6.75114 LUMO: -0.55239 factor:1 | 1 (-0.99270) | -1 | -1 |
| G: -6289.33611 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12556.08310 HOMO: -6.49536 LUMO: -0.25307 factor:1 | 1 (-2.38130) | -1 | -1 |
| G: -6289.33611 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.54884 HOMO: -6.48992 LUMO: -0.25034 factor:1 | 1 (-1.84703) | -1 | -1 |
| G: -6289.33611 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.59148 HOMO: -6.52801 LUMO: -0.28028 factor:1 | 1 (-1.88967) | -1 | -1 |
| G: -6289.33611 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.59877 HOMO: -7.22462 LUMO: 0.52518 factor:1 | 1 (-1.89696) | -1 | -1 |
| G: -6289.33611 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.65365 HOMO: -6.59332 LUMO: -0.27211 factor:1 | 1 (-1.95185) | -1 | -1 |
| G: -6289.33611 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.71919 HOMO: -6.57427 LUMO: -0.16871 factor:1 | 1 (-1.01738) | -1 | -1 |
| G: -6289.33611 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.70757 HOMO: -6.71033 LUMO: 1.59187 factor:1 | 1 (-1.00576) | -1 | -1 |
| G: -6289.33611 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.61769 HOMO: -6.72121 LUMO: 2.00004 factor:1 | 1 (-0.91588) | -1 | -1 |
| G: -6289.33611 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.72281 HOMO: -6.61509 LUMO: 1.55921 factor:1 | 1 (-1.02100) | -1 | -1 |
| G: -6289.33611 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.70787 HOMO: -6.55250 LUMO: 1.73064 factor:1 | 1 (-1.00606) | -1 | -1 |
| G: -6289.33611 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.46174 HOMO: -6.66135 LUMO: 2.02181 factor:1 | 1 (-0.75993) | -1 | -1 |
| G: -6289.33611 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12556.68480 HOMO: -6.84911 LUMO: 1.98099 factor:1 | 1 (-2.98299) | -1 | -1 |
| G: -6289.33611 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.88345 HOMO: -6.66679 LUMO: 1.98371 factor:1 | 1 (-2.18165) | -1 | -1 |
| G: -6289.33611 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.54762 HOMO: -6.67495 LUMO: 2.04085 factor:1 | 1 (-0.84581) | -1 | -1 |
| G: -6289.33611 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.96054 HOMO: -6.89809 LUMO: 1.95106 factor:1 | 1 (-2.25874) | -1 | -1 |
| G: -6289.33611 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12556.01973 HOMO: -6.50352 LUMO: 1.88847 factor:1 | 1 (-2.31792) | -1 | -1 |
| G: -6289.33611 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.38168 HOMO: -6.93618 LUMO: 2.00004 factor:1 | 1 (-1.67987) | -1 | -1 |
| G: -6289.33611 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.54633 HOMO: -6.50896 LUMO: 1.73609 factor:1 | 1 (-1.84452) | -1 | -1 |
| G: -6289.33611 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.49572 HOMO: -6.69672 LUMO: 2.37283 factor:1 | 1 (-1.79391) | -1 | -1 |
| G: -6289.33611 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.54122 HOMO: -6.65591 LUMO: 2.20684 factor:1 | 1 (-0.83942) | -1 | -1 |
| G: -6289.33611 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.57461 HOMO: -6.23957 LUMO: 1.78507 factor:1 | 1 (-0.87281) | -1 | -1 |
| G: -6289.33611 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.67320 HOMO: -6.35114 LUMO: 1.92112 factor:1 | 1 (-0.97139) | -1 | -1 |
| G: -6289.33611 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.86651 HOMO: -6.53617 LUMO: 1.75241 factor:1 | 1 (-1.16470) | -1 | -1 |
| G: -6289.33611 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.87571 HOMO: -6.60420 LUMO: 1.78779 factor:1 | 1 (-1.17390) | -1 | -1 |
| G: -6289.33611 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.81622 HOMO: -7.40422 LUMO: -0.97145 factor:1 | 1 (-1.11442) | -1 | -1 |
| G: -6289.33611 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.97568 HOMO: -6.80013 LUMO: -0.69117 factor:1 | 1 (-1.27387) | -1 | -1 |
| G: -6289.33611 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.78226 HOMO: -6.68040 LUMO: -0.47076 factor:1 | 1 (-1.08046) | -1 | -1 |
| G: -6289.33611 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.38744 HOMO: -7.20285 LUMO: -0.66124 factor:1 | 1 (-1.68564) | -1 | -1 |
| G: -6289.33611 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.52130 HOMO: -6.82734 LUMO: -0.60137 factor:1 | 1 (-1.81949) | -1 | -1 |
| G: -6289.33611 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.29925 HOMO: -7.18653 LUMO: 0.59321 factor:1 | 1 (-1.59744) | -1 | -1 |
| G: -6289.33611 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.67130 HOMO: -7.29265 LUMO: 0.48164 factor:1 | 1 (-0.96949) | -1 | -1 |
| G: -6289.33611 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.65012 HOMO: -6.63414 LUMO: -0.25034 factor:1 | 1 (-0.94832) | -1 | -1 |
| G: -6289.33611 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.82164 HOMO: -7.20285 LUMO: 0.53879 factor:1 | 1 (-1.11983) | -1 | -1 |
| G: -6289.33611 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.69924 HOMO: -6.46815 LUMO: -0.21769 factor:1 | 1 (-0.99743) | -1 | -1 |
| G: -6289.33611 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.75658 HOMO: -6.57971 LUMO: -0.18776 factor:1 | 1 (-1.05477) | -1 | -1 |
| G: -6289.33611 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.69048 HOMO: -6.90897 LUMO: 1.91296 factor:1 | 1 (-0.98867) | -1 | -1 |
| G: -6289.33611 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.39765 HOMO: -6.67495 LUMO: 2.04358 factor:1 | 1 (-1.69584) | -1 | -1 |
| G: -6289.33611 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.60682 HOMO: -6.94162 LUMO: 1.73881 factor:1 | 1 (-1.90501) | -1 | -1 |
| G: -6289.33611 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.54734 HOMO: -6.73482 LUMO: 1.95922 factor:1 | 1 (-1.84553) | -1 | -1 |
| G: -6289.33611 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.77078 HOMO: -6.70489 LUMO: 2.04358 factor:1 | 1 (-1.06897) | -1 | -1 |
| G: -6289.33611 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.25792 HOMO: -7.04231 LUMO: 1.79323 factor:1 | 1 (-1.55611) | -1 | -1 |
| G: -6289.33611 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.38347 HOMO: -6.68584 LUMO: 1.60275 factor:1 | 1 (-1.68166) | -1 | -1 |
| G: -6289.33611 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.34524 HOMO: -6.40556 LUMO: 1.45581 factor:1 | 1 (-1.64343) | -1 | -1 |
| G: -6289.33611 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.41803 HOMO: -6.94979 LUMO: 2.16603 factor:1 | 1 (-1.71622) | -1 | -1 |
| G: -6289.33611 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.18524 HOMO: -6.84911 LUMO: 1.89935 factor:1 | 1 (-1.48343) | -1 | -1 |
| G: -6289.33611 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.19827 HOMO: -6.22052 LUMO: 1.57282 factor:1 | 1 (-1.49646) | -1 | -1 |
| G: -6289.33611 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.47436 HOMO: -6.51168 LUMO: 2.10072 factor:1 | 1 (-1.77255) | -1 | -1 |
| G: -6289.33611 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12556.70061 HOMO: -7.03686 LUMO: 2.12249 factor:1 | 1 (-2.99880) | -1 | -1 |
| G: -6289.33611 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.93363 HOMO: -6.84094 LUMO: 1.63268 factor:1 | 1 (-2.23182) | -1 | -1 |
| G: -6289.33611 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.71648 HOMO: -6.75387 LUMO: 1.72248 factor:1 | 1 (-2.01468) | -1 | -1 |
| G: -6289.33611 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12556.07206 HOMO: -6.86271 LUMO: 1.68711 factor:1 | 1 (-2.37025) | -1 | -1 |
| G: -6289.33611 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.70281 HOMO: -6.84094 LUMO: 2.02997 factor:1 | 1 (-1.00100) | -1 | -1 |
| G: -6289.33611 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12556.21807 HOMO: -6.80557 LUMO: 2.02725 factor:1 | 1 (-2.51626) | -1 | -1 |
| G: -6289.33611 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.67232 HOMO: -6.38651 LUMO: 1.53472 factor:1 | 1 (-1.97051) | -1 | -1 |
| G: -6289.33611 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.76468 HOMO: -7.51306 LUMO: 0.28572 factor:1 | 1 (-1.06288) | -1 | -1 |
| G: -6289.33611 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.61064 HOMO: -6.97972 LUMO: -0.74287 factor:1 | 1 (-0.90883) | -1 | -1 |
| G: -6289.33611 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.39020 HOMO: -6.83822 LUMO: -0.65852 factor:1 | 1 (-0.68839) | -1 | -1 |
| G: -6289.33611 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.53635 HOMO: -6.71305 LUMO: -0.49525 factor:1 | 1 (-0.83455) | -1 | -1 |
| G: -6289.33611 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.68678 HOMO: -6.60692 LUMO: -0.22313 factor:1 | 1 (-0.98497) | -1 | -1 |
| G: -6289.33611 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.26336 HOMO: -7.20013 LUMO: 0.55239 factor:1 | 1 (-1.56155) | -1 | -1 |
| G: -6289.33611 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.31811 HOMO: -6.60420 LUMO: -0.28028 factor:1 | 1 (-1.61630) | -1 | -1 |
| G: -6289.33611 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.49142 HOMO: -6.69128 LUMO: -0.30477 factor:1 | 1 (-1.78961) | -1 | -1 |
| G: -6289.33611 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.65447 HOMO: -6.65591 LUMO: -0.25579 factor:1 | 1 (-1.95266) | -1 | -1 |
| G: -6289.33611 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.40562 HOMO: -6.69128 LUMO: 1.70888 factor:1 | 1 (-1.70381) | -1 | -1 |
| G: -6289.33611 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.35355 HOMO: -6.50080 LUMO: 1.87759 factor:1 | 1 (-0.65174) | -1 | -1 |
| G: -6289.33611 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.34291 HOMO: -6.85727 LUMO: 1.99187 factor:1 | 1 (-0.64110) | -1 | -1 |
| G: -6289.33611 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12556.55971 HOMO: -6.58788 LUMO: 1.79051 factor:1 | 1 (-2.85790) | -1 | -1 |
| G: -6289.33611 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.65673 HOMO: -6.64230 LUMO: 2.16058 factor:1 | 1 (-1.95492) | -1 | -1 |
| G: -6289.33611 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.31529 HOMO: -6.58788 LUMO: 2.10616 factor:1 | 1 (-0.61348) | -1 | -1 |
| G: -6289.33611 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.92762 HOMO: -7.01782 LUMO: 2.13609 factor:1 | 1 (-2.22581) | -1 | -1 |
| G: -6289.33611 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12556.04014 HOMO: -6.31304 LUMO: 2.31841 factor:1 | 1 (-2.33833) | -1 | -1 |
| G: -6289.33611 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.26508 HOMO: -6.94979 LUMO: 2.07895 factor:1 | 1 (-1.56327) | -1 | -1 |
| G: -6289.33611 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.28399 HOMO: -6.88992 LUMO: 2.28031 factor:1 | 1 (-1.58218) | -1 | -1 |
| G: -6289.33611 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.66449 HOMO: -6.66407 LUMO: 2.07623 factor:1 | 1 (-0.96268) | -1 | -1 |
| G: -6289.33611 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.76854 HOMO: -6.52529 LUMO: 1.70071 factor:1 | 1 (-2.06673) | -1 | -1 |
| G: -6289.33611 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.67120 HOMO: -6.58788 LUMO: 1.57282 factor:1 | 1 (-1.96940) | -1 | -1 |
| G: -6289.33611 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12556.20950 HOMO: -6.55250 LUMO: 1.95378 factor:1 | 1 (-2.50769) | -1 | -1 |
| G: -6289.33611 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.89138 HOMO: -6.24773 LUMO: 1.77962 factor:1 | 1 (-1.18957) | -1 | -1 |
| G: -6289.33611 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.41596 HOMO: -6.31304 LUMO: 2.18507 factor:1 | 1 (-1.71415) | -1 | -1 |
| G: -6289.33611 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.24475 HOMO: -6.18243 LUMO: 2.01636 factor:1 | 1 (-1.54294) | -1 | -1 |
| G: -6289.33611 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.00872 HOMO: -6.99877 LUMO: 2.14970 factor:1 | 1 (-1.30691) | -1 | -1 |
| G: -6289.33611 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.95936 HOMO: -6.72665 LUMO: 2.07079 factor:1 | 1 (-1.25755) | -1 | -1 |
| G: -6289.33611 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.92877 HOMO: -6.36202 LUMO: 2.17419 factor:1 | 1 (-1.22696) | -1 | -1 |
| G: -6289.33611 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.12213 HOMO: -6.78652 LUMO: 2.05718 factor:1 | 1 (-1.42033) | -1 | -1 |
| G: -6289.33611 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.97280 HOMO: -6.87360 LUMO: 2.34290 factor:1 | 1 (-1.27099) | -1 | -1 |
| G: -6289.33611 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.79601 HOMO: -6.62053 LUMO: 1.89391 factor:1 | 1 (-1.09420) | -1 | -1 |
| G: -6289.33611 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.84499 HOMO: -6.58788 LUMO: 1.83133 factor:1 | 1 (-1.14318) | -1 | -1 |
| G: -6289.33611 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.54622 HOMO: -7.08584 LUMO: 1.91568 factor:1 | 1 (-1.84441) | 1 | 1 |
| G: -6289.33611 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.50007 HOMO: -6.56883 LUMO: 1.81228 factor:1 | 1 (-1.79826) | -1 | -1 |
| G: -6289.33611 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.36304 HOMO: -6.66135 LUMO: 1.92384 factor:1 | 1 (-1.66123) | -1 | -1 |
| G: -6289.33611 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.65281 HOMO: -6.64502 LUMO: 2.15786 factor:1 | 1 (-1.95100) | -1 | -1 |
| G: -6289.33611 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.49479 HOMO: -6.71305 LUMO: 1.91840 factor:1 | 1 (-1.79299) | -1 | -1 |
| G: -6289.33611 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.53417 HOMO: -6.44094 LUMO: 1.74425 factor:1 | 1 (-1.83236) | -1 | -1 |
| G: -6289.33611 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.63851 HOMO: -6.51985 LUMO: 1.84221 factor:1 | 1 (-0.93670) | -1 | -1 |
| G: -6289.33611 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.46551 HOMO: -6.63414 LUMO: -0.24762 factor:1 | 1 (-1.76371) | -1 | -1 |
| G: -6289.33611 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.61232 HOMO: -6.60420 LUMO: -0.22585 factor:1 | 1 (-1.91051) | -1 | -1 |
| G: -6289.33611 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.45950 HOMO: -7.19741 LUMO: 0.58232 factor:1 | 1 (-1.75769) | -1 | -1 |
| G: -6289.33611 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.42383 HOMO: -6.77019 LUMO: -0.56872 factor:1 | 1 (-1.72202) | -1 | -1 |
| G: -6289.33611 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.69110 HOMO: -7.46136 LUMO: 0.28844 factor:1 | 1 (-1.98929) | -1 | -1 |
| G: -6289.33611 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.57724 HOMO: -6.60420 LUMO: -0.54151 factor:1 | 1 (-1.87544) | -1 | -1 |
| G: -6289.33611 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.68906 HOMO: -6.53890 LUMO: -0.46531 factor:1 | 1 (-1.98725) | -1 | -1 |
| G: -6289.33611 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.50249 HOMO: -6.81645 LUMO: -0.57144 factor:1 | 1 (-1.80069) | -1 | -1 |
| G: -6289.33611 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.61806 HOMO: -7.48041 LUMO: 0.28572 factor:1 | 1 (-1.91625) | -1 | -1 |
| G: -6289.33611 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.42007 HOMO: -6.75659 LUMO: -0.45715 factor:1 | 1 (-1.71826) | -1 | -1 |
| G: -6289.33611 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.34780 HOMO: -6.66135 LUMO: -0.41906 factor:1 | 1 (-1.64599) | -1 | -1 |
| G: -6289.33611 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.72836 HOMO: -6.55794 LUMO: -0.27483 factor:1 | 1 (-1.02655) | -1 | -1 |
| G: -6289.33611 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.44113 HOMO: -7.07496 LUMO: -0.63403 factor:1 | 1 (-1.73932) | -1 | -1 |
| G: -6289.33611 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.36889 HOMO: -7.12394 LUMO: 0.53334 factor:1 | 1 (-1.66708) | -1 | -1 |
| G: -6289.33611 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.38940 HOMO: -6.53617 LUMO: -0.25579 factor:1 | 1 (-1.68760) | -1 | -1 |
| G: -6289.33611 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.48356 HOMO: -6.50896 LUMO: -0.25034 factor:1 | 1 (-1.78175) | -1 | -1 |
| G: -6289.33611 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.59907 HOMO: -7.17564 LUMO: -0.68573 factor:1 | 1 (-1.89726) | -1 | -1 |
| G: -6289.33611 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.71172 HOMO: -6.53617 LUMO: -0.30749 factor:1 | 1 (-2.00991) | -1 | -1 |
| G: -6289.33611 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.87701 HOMO: -6.55522 LUMO: -0.30749 factor:1 | 1 (-1.17521) | -1 | -1 |
| G: -6289.33611 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.32080 HOMO: -7.05591 LUMO: -0.71022 factor:1 | 1 (-1.61900) | -1 | -1 |
| G: -6289.33611 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.98714 HOMO: -7.17564 LUMO: -0.69933 factor:1 | 1 (-1.28533) | -1 | -1 |
| G: -6289.33611 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.27427 HOMO: -6.78380 LUMO: -0.67756 factor:1 | 1 (-1.57246) | -1 | -1 |
| G: -6289.33611 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.02586 HOMO: -6.62325 LUMO: 2.02725 factor:1 | 1 (-1.32405) | -1 | -1 |
| G: -6289.33611 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.39237 HOMO: -6.63414 LUMO: 1.91296 factor:1 | 1 (-1.69056) | -1 | -1 |
| G: -6289.33611 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.46897 HOMO: -6.83278 LUMO: 1.65717 factor:1 | 1 (-1.76716) | -1 | -1 |
| G: -6289.33611 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.46252 HOMO: -6.66407 LUMO: 1.95650 factor:1 | 1 (-1.76071) | -1 | -1 |
| G: -6289.33611 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.44023 HOMO: -6.61237 LUMO: 2.11432 factor:1 | 1 (-1.73843) | -1 | -1 |
| G: -6289.33611 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.04311 HOMO: -6.62053 LUMO: 2.09256 factor:1 | 1 (-1.34130) | -1 | -1 |
| G: -6289.33611 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.00779 HOMO: -6.78652 LUMO: 2.13609 factor:1 | 1 (-1.30598) | -1 | -1 |
| G: -6289.33611 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.26616 HOMO: -6.94707 LUMO: 1.81772 factor:1 | 1 (-1.56436) | -1 | -1 |
| G: -6289.33611 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.14711 HOMO: -6.85183 LUMO: 2.12793 factor:1 | 1 (-1.44531) | -1 | -1 |
| G: -6289.33611 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.10635 HOMO: -6.81101 LUMO: 1.83949 factor:1 | 1 (-1.40454) | -1 | -1 |
| G: -6289.33611 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.73323 HOMO: -6.98788 LUMO: 2.16058 factor:1 | 1 (-1.03142) | -1 | -1 |
| G: -6289.33611 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.92801 HOMO: -6.62869 LUMO: 2.00820 factor:1 | 1 (-1.22620) | -1 | -1 |
| G: -6289.33611 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.91440 HOMO: -6.34025 LUMO: 2.25855 factor:1 | 1 (-1.21259) | -1 | -1 |
| G: -6289.33611 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.85573 HOMO: -6.01372 LUMO: 2.01636 factor:1 | 1 (-1.15393) | -1 | -1 |
| G: -6289.33611 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.48422 HOMO: -6.89264 LUMO: 2.27487 factor:1 | 1 (-0.78241) | -1 | -1 |
| G: -6289.33611 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.99331 HOMO: -6.53073 LUMO: 2.20684 factor:1 | 1 (-1.29151) | -1 | -1 |
| G: -6289.33611 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.62117 HOMO: -6.83278 LUMO: 1.53744 factor:1 | 1 (-0.91936) | -1 | -1 |
| G: -6289.33611 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.35904 HOMO: -6.41917 LUMO: 1.82316 factor:1 | 1 (-1.65723) | -1 | -1 |
| G: -6289.33611 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.89507 HOMO: -6.56339 LUMO: 1.63813 factor:1 | 1 (-2.19326) | -1 | -1 |
| G: -6289.33611 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.85657 HOMO: -6.88992 LUMO: 1.65173 factor:1 | 1 (-2.15476) | -1 | -1 |
| G: -6289.33611 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12556.42352 HOMO: -6.63141 LUMO: 1.92112 factor:1 | 1 (-2.72171) | -1 | -1 |
| G: -6289.33611 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12556.25546 HOMO: -6.83822 LUMO: 1.88847 factor:1 | 1 (-2.55365) | -1 | -1 |
| G: -6289.33611 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.93594 HOMO: -6.84638 LUMO: 1.90480 factor:1 | 1 (-2.23414) | -1 | -1 |
| G: -6289.33611 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.54247 HOMO: -6.82462 LUMO: 1.70888 factor:1 | 1 (-1.84066) | -1 | -1 |
| G: -6289.33611 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.85921 HOMO: -6.82734 LUMO: 2.12521 factor:1 | 1 (-2.15740) | -1 | -1 |
| G: -6289.33611 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.81126 HOMO: -6.94435 LUMO: 1.87214 factor:1 | 1 (-2.10945) | -1 | -1 |
| G: -6289.33611 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12556.06357 HOMO: -6.98516 LUMO: 2.51433 factor:1 | 1 (-2.36176) | -1 | -1 |
| G: -6289.33611 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12556.39748 HOMO: -6.74026 LUMO: 2.15514 factor:1 | 1 (-2.69567) | -1 | -1 |
| G: -6289.33611 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12556.39677 HOMO: -6.93618 LUMO: 2.54426 factor:1 | 1 (-2.69496) | -1 | -1 |
| G: -6289.33611 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12556.55440 HOMO: -6.28583 LUMO: 2.53610 factor:1 | 1 (-2.85260) | -1 | -1 |
| G: -6289.33611 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.91496 HOMO: -6.56883 LUMO: 1.94834 factor:1 | 1 (-2.21316) | -1 | -1 |
| G: -6289.33611 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12556.60692 HOMO: -7.08584 LUMO: 1.99187 factor:1 | 1 (-2.90511) | 1 | 1 |
| G: -6289.33611 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12556.45731 HOMO: -6.19059 LUMO: 1.99732 factor:1 | 1 (-2.75551) | -1 | -1 |
| G: -6289.33611 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.65442 HOMO: -6.78108 LUMO: 2.03813 factor:1 | 1 (-1.95261) | -1 | -1 |
| G: -6289.33611 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.88794 HOMO: -6.82189 LUMO: 1.77418 factor:1 | 1 (-2.18614) | -1 | -1 |
| G: -6289.33611 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12556.57098 HOMO: -6.45454 LUMO: 1.78779 factor:1 | 1 (-2.86917) | -1 | -1 |
| G: -6289.33611 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12556.44131 HOMO: -6.84366 LUMO: 1.77690 factor:1 | 1 (-2.73951) | -1 | -1 |
| G: -6289.33611 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12556.10923 HOMO: -6.74026 LUMO: 1.67622 factor:1 | 1 (-2.40742) | -1 | -1 |
| G: -6289.33611 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.84634 HOMO: -6.76475 LUMO: 2.40277 factor:1 | 1 (-2.14453) | -1 | -1 |
| G: -6289.33611 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.55694 HOMO: -6.65863 LUMO: 1.86670 factor:1 | 1 (-1.85514) | -1 | -1 |
| G: -6289.33611 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.41551 HOMO: -6.50080 LUMO: 1.93201 factor:1 | 1 (-0.71370) | -1 | -1 |
| G: -6289.33611 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.28005 HOMO: -6.34842 LUMO: 1.70888 factor:1 | 1 (-0.57824) | -1 | -1 |
| G: -6289.33611 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.44350 HOMO: -6.60692 LUMO: 2.20140 factor:1 | 1 (-1.74169) | -1 | -1 |
| G: -6289.33611 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.49281 HOMO: -6.74026 LUMO: 2.14970 factor:1 | 1 (-1.79100) | -1 | -1 |
| G: -6289.33611 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.68609 HOMO: -6.63686 LUMO: 2.17419 factor:1 | 1 (-1.98428) | -1 | -1 |
| G: -6289.33611 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.37958 HOMO: -6.81917 LUMO: 2.10072 factor:1 | 1 (-1.67777) | -1 | -1 |
| G: -6289.33611 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.79856 HOMO: -6.92802 LUMO: 2.04358 factor:1 | 1 (-1.09675) | -1 | -1 |
| G: -6289.33611 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.65685 HOMO: -6.56067 LUMO: -0.47620 factor:1 | 1 (-0.95504) | -1 | -1 |
| G: -6289.33611 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.57687 HOMO: -6.56611 LUMO: -0.77008 factor:1 | 1 (-0.87506) | -1 | -1 |
| G: -6289.33611 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.75309 HOMO: -6.78380 LUMO: -0.64763 factor:1 | 1 (-1.05128) | -1 | -1 |
| G: -6289.33611 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.74934 HOMO: -6.51985 LUMO: -0.24490 factor:1 | 1 (-1.04753) | -1 | -1 |
| G: -6289.33611 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.45328 HOMO: -6.52529 LUMO: -0.27483 factor:1 | 1 (-0.75147) | -1 | -1 |
| G: -6289.33611 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12556.04680 HOMO: -7.10489 LUMO: -0.62586 factor:1 | 1 (-2.34500) | -1 | -1 |
| G: -6289.33611 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12556.48874 HOMO: -7.18108 LUMO: 0.48980 factor:1 | 1 (-2.78694) | -1 | -1 |
| G: -6289.33611 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.55527 HOMO: -7.14299 LUMO: -0.63947 factor:1 | 1 (-0.85346) | -1 | -1 |
| G: -6289.33611 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.89015 HOMO: -6.70761 LUMO: -0.54423 factor:1 | 1 (-2.18834) | -1 | -1 |
| G: -6289.33611 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.23318 HOMO: -7.32258 LUMO: -1.03675 factor:1 | 1 (-1.53138) | -1 | -1 |
| G: -6289.33611 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.55499 HOMO: -6.65046 LUMO: -0.41361 factor:1 | 1 (-1.85318) | -1 | -1 |
| G: -6289.33611 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12556.12569 HOMO: -6.76475 LUMO: -0.60137 factor:1 | 1 (-2.42388) | -1 | -1 |
| G: -6289.33611 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.77570 HOMO: -6.77836 LUMO: -0.54423 factor:1 | 1 (-2.07389) | -1 | -1 |
| G: -6289.33611 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.51722 HOMO: -7.52395 LUMO: 0.26395 factor:1 | 1 (-1.81541) | -1 | -1 |
| G: -6289.33611 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.43194 HOMO: -6.93890 LUMO: -0.72382 factor:1 | 1 (-1.73013) | -1 | -1 |
| G: -6289.33611 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.58217 HOMO: -6.72938 LUMO: -0.47348 factor:1 | 1 (-1.88036) | -1 | -1 |
| G: -6289.33611 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.21248 HOMO: -6.66951 LUMO: -0.40817 factor:1 | 1 (-1.51067) | -1 | -1 |
| G: -6289.33611 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.55833 HOMO: -6.60420 LUMO: -0.19320 factor:1 | 1 (-1.85652) | -1 | -1 |
| G: -6289.33611 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.85545 HOMO: -6.67495 LUMO: -0.27211 factor:1 | 1 (-2.15365) | -1 | -1 |
| G: -6289.33611 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.42883 HOMO: -7.23823 LUMO: -0.62858 factor:1 | 1 (-1.72703) | -1 | -1 |
| G: -6289.33611 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.27749 HOMO: -7.27088 LUMO: 0.53334 factor:1 | 1 (-0.57568) | -1 | -1 |
| G: -6289.33611 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.46408 HOMO: -7.20013 LUMO: 0.59049 factor:1 | 1 (-0.76227) | -1 | -1 |
| G: -6289.33611 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12553.99694 HOMO: -6.60148 LUMO: -0.20953 factor:1 | 1 (-0.29513) | -1 | -1 |
| G: -6289.33611 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.56631 HOMO: -6.69400 LUMO: -0.51974 factor:1 | 1 (-0.86451) | -1 | -1 |
| G: -6289.33611 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.33210 HOMO: -7.40422 LUMO: -0.98777 factor:1 | 1 (-1.63029) | -1 | -1 |
| G: -6289.33611 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.94101 HOMO: -6.88176 LUMO: -0.71022 factor:1 | 1 (-2.23920) | -1 | -1 |
| G: -6289.33611 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.48211 HOMO: -6.86271 LUMO: -0.59321 factor:1 | 1 (-1.78030) | -1 | -1 |
| G: -6289.33611 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.18861 HOMO: -6.73754 LUMO: -0.55239 factor:1 | 1 (-1.48680) | -1 | -1 |
| G: -6289.33611 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.86854 HOMO: -6.71033 LUMO: 1.57010 factor:1 | 1 (-2.16673) | -1 | -1 |
| G: -6289.33611 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.79665 HOMO: -6.69672 LUMO: 1.68711 factor:1 | 1 (-2.09484) | -1 | -1 |
| G: -6289.33611 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.95600 HOMO: -6.67495 LUMO: 2.03813 factor:1 | 1 (-2.25419) | -1 | -1 |
| G: -6289.33611 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.59431 HOMO: -6.54434 LUMO: 1.83677 factor:1 | 1 (-1.89250) | -1 | -1 |
| G: -6289.33611 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.42780 HOMO: -6.57155 LUMO: 1.77146 factor:1 | 1 (-1.72599) | -1 | -1 |
| G: -6289.33611 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.37030 HOMO: -6.76747 LUMO: 1.87759 factor:1 | 1 (-1.66849) | -1 | -1 |
| G: -6289.33611 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.71711 HOMO: -6.58243 LUMO: 1.61364 factor:1 | 1 (-2.01530) | -1 | -1 |
| G: -6289.33611 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.42543 HOMO: -6.61781 LUMO: 2.13881 factor:1 | 1 (-1.72362) | -1 | -1 |
| G: -6289.33611 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.78242 HOMO: -6.62597 LUMO: 2.00276 factor:1 | 1 (-2.08061) | -1 | -1 |
| G: -6289.33611 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.82971 HOMO: -7.01237 LUMO: 1.95922 factor:1 | 1 (-2.12790) | -1 | -1 |
| G: -6289.33611 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.97521 HOMO: -7.03959 LUMO: 2.16875 factor:1 | 1 (-2.27340) | -1 | -1 |
| G: -6289.33611 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.66103 HOMO: -6.83278 LUMO: 1.91296 factor:1 | 1 (-1.95922) | -1 | -1 |
| G: -6289.33611 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.51219 HOMO: -6.40012 LUMO: 1.95650 factor:1 | 1 (-0.81038) | -1 | -1 |
| G: -6289.33611 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.43222 HOMO: -6.50080 LUMO: 1.73337 factor:1 | 1 (-0.73041) | -1 | -1 |
| G: -6289.33611 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.61187 HOMO: -6.95795 LUMO: 2.28848 factor:1 | 1 (-0.91006) | -1 | -1 |
| G: -6289.33611 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.32040 HOMO: -6.63686 LUMO: 2.20140 factor:1 | 1 (-0.61860) | -1 | -1 |
| G: -6289.33611 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.59978 HOMO: -6.57427 LUMO: 1.87214 factor:1 | 1 (-0.89798) | -1 | -1 |
| G: -6289.33611 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.40179 HOMO: -6.38379 LUMO: 2.32113 factor:1 | 1 (-1.69998) | -1 | -1 |
| G: -6289.33611 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.97271 HOMO: -6.63958 LUMO: 2.04902 factor:1 | 1 (-2.27090) | -1 | -1 |
| G: -6289.33611 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.34627 HOMO: -6.70216 LUMO: 1.93201 factor:1 | 1 (-1.64447) | -1 | -1 |
| G: -6289.33611 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12556.20109 HOMO: -6.80557 LUMO: 2.23678 factor:1 | 1 (-2.49928) | -1 | -1 |
| G: -6289.33611 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.54625 HOMO: -6.72938 LUMO: 2.28304 factor:1 | 1 (-1.84444) | -1 | -1 |
| G: -6289.33611 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.88593 HOMO: -6.56067 LUMO: 1.66806 factor:1 | 1 (-2.18412) | -1 | -1 |
| G: -6289.33611 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.32987 HOMO: -6.95523 LUMO: 2.33474 factor:1 | 1 (-1.62806) | -1 | -1 |
| G: -6289.33611 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.18616 HOMO: -6.59876 LUMO: 2.30480 factor:1 | 1 (-1.48435) | -1 | -1 |
| G: -6289.33611 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.41874 HOMO: -6.87360 LUMO: 1.75786 factor:1 | 1 (-1.71693) | -1 | -1 |
| G: -6289.33611 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.47463 HOMO: -7.06408 LUMO: 1.99187 factor:1 | 1 (-1.77282) | 1 | 1 |
| G: -6289.33611 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.20216 HOMO: -6.95795 LUMO: 1.88847 factor:1 | 1 (-1.50035) | -1 | -1 |
| G: -6289.33611 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.10755 HOMO: -6.85455 LUMO: 1.63813 factor:1 | 1 (-1.40574) | -1 | -1 |
| G: -6289.33611 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.89584 HOMO: -7.09129 LUMO: 2.31569 factor:1 | 1 (-1.19404) | 1 | 1 |
| G: -6289.33611 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.05076 HOMO: -6.91441 LUMO: 1.68983 factor:1 | 1 (-1.34895) | -1 | -1 |
| G: -6289.33611 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.35009 HOMO: -6.89809 LUMO: 2.23678 factor:1 | 1 (-0.64828) | -1 | -1 |
| G: -6289.33611 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.53429 HOMO: -6.78652 LUMO: 1.98371 factor:1 | 1 (-0.83248) | -1 | -1 |
| G: -6289.33611 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.68240 HOMO: -6.94707 LUMO: 2.23678 factor:1 | 1 (-0.98059) | -1 | -1 |
| G: -6289.33611 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.84537 HOMO: -7.07224 LUMO: 2.13337 factor:1 | 1 (-1.14356) | 1 | 1 |
| G: -6289.33611 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.72025 HOMO: -6.94979 LUMO: 2.28031 factor:1 | 1 (-1.01844) | -1 | -1 |
| G: -6289.33611 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.33523 HOMO: -6.60965 LUMO: 2.20412 factor:1 | 1 (-0.63343) | -1 | -1 |
| G: -6289.33611 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.41393 HOMO: -6.87360 LUMO: 2.40277 factor:1 | 1 (-0.71212) | -1 | -1 |
| G: -6289.33611 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.74822 HOMO: -6.92802 LUMO: 1.89663 factor:1 | 1 (-1.04641) | -1 | -1 |
| G: -6289.33611 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.38854 HOMO: -6.88448 LUMO: 2.02725 factor:1 | 1 (-0.68673) | -1 | -1 |
| G: -6289.33611 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.62724 HOMO: -6.69128 LUMO: 1.55105 factor:1 | 1 (-0.92543) | -1 | -1 |
| G: -6289.33611 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.29366 HOMO: -6.54978 LUMO: 1.93201 factor:1 | 1 (-0.59185) | -1 | -1 |
| G: -6289.33611 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.77864 HOMO: -6.19331 LUMO: 1.46941 factor:1 | 1 (-1.07684) | -1 | -1 |
| G: -6289.33611 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.46397 HOMO: -6.55794 LUMO: 1.89663 factor:1 | 1 (-0.76216) | -1 | -1 |
| G: -6289.33611 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.63271 HOMO: -6.07630 LUMO: 1.94289 factor:1 | 1 (-0.93090) | -1 | -1 |
| G: -6289.33611 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.62936 HOMO: -7.46408 LUMO: 0.31565 factor:1 | 1 (-0.92755) | -1 | -1 |
| G: -6289.33611 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.30228 HOMO: -6.63958 LUMO: -0.61770 factor:1 | 1 (-0.60047) | -1 | -1 |
| G: -6289.33611 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.20144 HOMO: -6.81101 LUMO: -0.57960 factor:1 | 1 (-0.49963) | -1 | -1 |
| G: -6289.33611 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.38955 HOMO: -6.74298 LUMO: -0.57960 factor:1 | 1 (-0.68774) | -1 | -1 |
| G: -6289.33611 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.42691 HOMO: -6.63686 LUMO: -0.42994 factor:1 | 1 (-0.72510) | -1 | -1 |
| G: -6289.33611 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.53001 HOMO: -6.60965 LUMO: -0.41089 factor:1 | 1 (-0.82821) | -1 | -1 |
| G: -6289.33611 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.44019 HOMO: -6.60692 LUMO: -0.80274 factor:1 | 1 (-0.73838) | -1 | -1 |
| G: -6289.33611 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.25118 HOMO: -6.58788 LUMO: -0.78097 factor:1 | 1 (-0.54937) | -1 | -1 |
| G: -6289.33611 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.74692 HOMO: -6.67767 LUMO: -0.48436 factor:1 | 1 (-1.04511) | -1 | -1 |
| G: -6289.33611 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.66773 HOMO: -6.63141 LUMO: -0.40545 factor:1 | 1 (-0.96592) | -1 | -1 |
| G: -6289.33611 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.80055 HOMO: -6.62053 LUMO: -0.83811 factor:1 | 1 (-1.09874) | -1 | -1 |
| G: -6289.33611 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.66735 HOMO: -6.59604 LUMO: -0.35375 factor:1 | 1 (-0.96554) | -1 | -1 |
| G: -6289.33611 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.41320 HOMO: -6.34297 LUMO: -0.39729 factor:1 | 1 (-0.71139) | -1 | -1 |
| G: -6289.33611 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.52378 HOMO: -6.67223 LUMO: 1.97827 factor:1 | 1 (-0.82197) | -1 | -1 |
| G: -6289.33611 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.56373 HOMO: -6.40012 LUMO: 1.89935 factor:1 | 1 (-0.86192) | -1 | -1 |
| G: -6289.33611 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.19877 HOMO: -6.74842 LUMO: 1.97283 factor:1 | 1 (-0.49696) | -1 | -1 |
| G: -6289.33611 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.26500 HOMO: -6.76747 LUMO: 2.17147 factor:1 | 1 (-0.56319) | -1 | -1 |
| G: -6289.33611 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.42604 HOMO: -6.72121 LUMO: 1.55649 factor:1 | 1 (-0.72423) | -1 | -1 |
| G: -6289.33611 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.46571 HOMO: -6.97700 LUMO: 2.04085 factor:1 | 1 (-0.76391) | -1 | -1 |
| G: -6289.33611 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.56142 HOMO: -7.06680 LUMO: 2.04085 factor:1 | 1 (-0.85961) | 1 | 1 |
| G: -6289.33611 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.54381 HOMO: -7.09673 LUMO: 2.35106 factor:1 | 1 (-0.84200) | 1 | 1 |
| G: -6289.33611 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.67834 HOMO: -6.83006 LUMO: 2.14970 factor:1 | 1 (-0.97654) | -1 | -1 |
| G: -6289.33611 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.42332 HOMO: -6.72665 LUMO: 2.20140 factor:1 | 1 (-0.72151) | -1 | -1 |
| G: -6289.33611 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.46095 HOMO: -6.77291 LUMO: 2.34562 factor:1 | 1 (-0.75914) | -1 | -1 |
| G: -6289.33611 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.10170 HOMO: -6.73754 LUMO: 2.00276 factor:1 | 1 (-1.39989) | -1 | -1 |
| G: -6289.33611 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.20706 HOMO: -7.04231 LUMO: 1.92112 factor:1 | 1 (-1.50525) | -1 | -1 |
| G: -6289.33611 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.30053 HOMO: -6.83822 LUMO: 1.72248 factor:1 | 1 (-1.59872) | -1 | -1 |
| G: -6289.33611 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.34951 HOMO: -6.57971 LUMO: 2.16603 factor:1 | 1 (-1.64770) | -1 | -1 |
| G: -6289.33611 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.98787 HOMO: -6.80013 LUMO: 1.88575 factor:1 | 1 (-1.28606) | -1 | -1 |
| G: -6289.33611 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.99492 HOMO: -6.93618 LUMO: 2.18235 factor:1 | 1 (-1.29311) | -1 | -1 |
| G: -6289.33611 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.35988 HOMO: -6.54706 LUMO: 1.91024 factor:1 | 1 (-1.65807) | -1 | -1 |
| G: -6289.33611 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.15843 HOMO: -7.06952 LUMO: 2.18507 factor:1 | 1 (-1.45663) | 1 | 1 |
| G: -6289.33611 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.70421 HOMO: -7.05047 LUMO: 1.82044 factor:1 | 1 (-2.00240) | -1 | -1 |
| G: -6289.33611 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.80133 HOMO: -6.87632 LUMO: 1.92657 factor:1 | 1 (-2.09952) | -1 | -1 |
| G: -6289.33611 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12556.57601 HOMO: -6.58788 LUMO: 1.91568 factor:1 | 1 (-2.87420) | -1 | -1 |
| G: -6289.33611 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12556.55519 HOMO: -7.17292 LUMO: 1.90752 factor:1 | 1 (-2.85339) | 1 | 1 |
| G: -6289.33611 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.83722 HOMO: -6.93890 LUMO: 1.80684 factor:1 | 1 (-2.13541) | -1 | -1 |
| G: -6289.33611 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12556.40556 HOMO: -7.10761 LUMO: 2.20956 factor:1 | 1 (-2.70375) | 1 | 1 |
| G: -6289.33611 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12556.27206 HOMO: -6.85727 LUMO: 2.13609 factor:1 | 1 (-2.57025) | -1 | -1 |
| G: -6289.33611 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.60386 HOMO: -6.64502 LUMO: 1.38506 factor:1 | 1 (-1.90205) | -1 | -1 |
| G: -6289.33611 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12556.09045 HOMO: -6.87360 LUMO: 1.15648 factor:1 | 1 (-2.38864) | -1 | -1 |
| G: -6289.33611 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.45866 HOMO: -6.67223 LUMO: 2.07351 factor:1 | 1 (-1.75685) | -1 | -1 |
| G: -6289.33611 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.46579 HOMO: -6.29671 LUMO: 2.43270 factor:1 | 1 (-1.76398) | -1 | -1 |
| G: -6289.33611 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.36274 HOMO: -6.90897 LUMO: 2.28848 factor:1 | 1 (-1.66093) | -1 | -1 |
| G: -6289.33611 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.71178 HOMO: -7.04231 LUMO: 1.70071 factor:1 | 1 (-2.00997) | -1 | -1 |
| G: -6289.33611 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.39857 HOMO: -6.69944 LUMO: 1.94834 factor:1 | 1 (-1.69677) | -1 | -1 |
| G: -6289.33611 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.61440 HOMO: -6.56067 LUMO: 2.20956 factor:1 | 1 (-0.91259) | -1 | -1 |
| G: -6289.33611 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.61851 HOMO: -6.65046 LUMO: 2.06807 factor:1 | 1 (-0.91670) | -1 | -1 |
| G: -6289.33611 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.30334 HOMO: -7.08584 LUMO: 1.98915 factor:1 | 1 (-0.60153) | 1 | 1 |
| G: -6289.33611 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.71309 HOMO: -6.69400 LUMO: 2.09256 factor:1 | 1 (-1.01128) | -1 | -1 |
| G: -6289.33611 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.50000 HOMO: -6.62869 LUMO: 2.16331 factor:1 | 1 (-0.79819) | -1 | -1 |
| G: -6289.33611 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.29050 HOMO: -6.85183 LUMO: 2.16058 factor:1 | 1 (-0.58869) | -1 | -1 |
| G: -6289.33611 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.54531 HOMO: -6.54706 LUMO: 1.92384 factor:1 | 1 (-0.84350) | -1 | -1 |
| G: -6289.33611 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.39230 HOMO: -6.84366 LUMO: 2.48984 factor:1 | 1 (-0.69049) | -1 | -1 |
| G: -6289.33611 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.87047 HOMO: -6.77291 LUMO: 2.46263 factor:1 | 1 (-2.16867) | -1 | -1 |
| G: -6289.33611 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12556.40550 HOMO: -7.01782 LUMO: 2.31025 factor:1 | 1 (-2.70370) | -1 | -1 |
| G: -6289.33611 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.53828 HOMO: -6.94707 LUMO: 2.29664 factor:1 | 1 (-1.83647) | -1 | -1 |
| G: -6289.33611 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12556.52069 HOMO: -6.64230 LUMO: 1.97283 factor:1 | 1 (-2.81888) | -1 | -1 |
| G: -6289.33611 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12556.22874 HOMO: -6.47359 LUMO: 2.20412 factor:1 | 1 (-2.52693) | -1 | -1 |
| G: -6289.33611 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.26968 HOMO: -6.90625 LUMO: 1.92384 factor:1 | 1 (-0.56787) | -1 | -1 |
| G: -6289.33611 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.48653 HOMO: -7.17020 LUMO: 2.06807 factor:1 | 1 (-0.78472) | 1 | 1 |
| G: -6289.33611 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.27308 HOMO: -6.65046 LUMO: 2.20956 factor:1 | 1 (-0.57128) | -1 | -1 |
| G: -6289.33611 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.87967 HOMO: -7.07496 LUMO: 1.82861 factor:1 | 1 (-2.17786) | 1 | 1 |
| G: -6289.33611 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.10967 HOMO: -6.83006 LUMO: 2.14970 factor:1 | 1 (-1.40786) | -1 | -1 |
| G: -6289.33611 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.28453 HOMO: -6.92802 LUMO: 1.99187 factor:1 | 1 (-1.58272) | -1 | -1 |
| G: -6289.33611 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12556.05744 HOMO: -6.69672 LUMO: 2.36739 factor:1 | 1 (-2.35564) | -1 | -1 |
| G: -6289.33611 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.19008 HOMO: -7.13755 LUMO: 2.00276 factor:1 | 1 (-1.48827) | 1 | 1 |
| G: -6289.33611 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.80177 HOMO: -6.92530 LUMO: 2.25582 factor:1 | 1 (-2.09996) | -1 | -1 |
| G: -6289.33611 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12554.96692 HOMO: -6.77564 LUMO: 1.97827 factor:1 | 1 (-1.26511) | -1 | -1 |
| G: -6289.33611 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.46219 HOMO: -6.87904 LUMO: 1.60003 factor:1 | 1 (-1.76039) | -1 | -1 |
| G: -6289.33611 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.51469 HOMO: -6.62869 LUMO: 1.90480 factor:1 | 1 (-1.81288) | -1 | -1 |
| G: -6289.33611 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.28654 HOMO: -6.71033 LUMO: 1.54833 factor:1 | 1 (-1.58474) | -1 | -1 |
| G: -6289.33611 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.33955 HOMO: -6.74298 LUMO: 1.47486 factor:1 | 1 (-1.63774) | -1 | -1 |
| G: -6289.33611 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.43308 HOMO: -6.77019 LUMO: 1.90480 factor:1 | 1 (-1.73127) | -1 | -1 |
| G: -6289.33611 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12555.27237 HOMO: -6.70489 LUMO: 1.99459 factor:1 | 1 (-1.57056) | -1 | -1 |