乙二醇作为反应物的反应表19-5

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: -6257.41721 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.35355 HOMO: -6.91169 LUMO: -0.53879 factor:1 | 1 (-1.57064) | -1 | -1 |
| G: -6257.41721 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.95860 HOMO: -7.29809 LUMO: 2.83543 factor:1 | 1 (-1.17570) | 1 | -1 |
| G: -6257.41721 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.99852 HOMO: -6.86543 LUMO: -0.70205 factor:1 | 1 (-1.21561) | -1 | -1 |
| G: -6257.41721 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.40917 HOMO: -7.47769 LUMO: 0.31293 factor:1 | 1 (-1.62626) | -1 | -1 |
| G: -6257.41721 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.53524 HOMO: -6.63141 LUMO: -0.55511 factor:1 | 1 (-1.75233) | -1 | -1 |
| G: -6257.41721 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.31306 HOMO: -6.68856 LUMO: -0.30205 factor:1 | 1 (-1.53015) | -1 | -1 |
| G: -6257.41721 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.30677 HOMO: -7.22190 LUMO: 0.53334 factor:1 | 1 (-1.52386) | -1 | -1 |
| G: -6257.41721 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.20693 HOMO: -6.66407 LUMO: -0.27756 factor:1 | 1 (-1.42403) | -1 | -1 |
| G: -6257.41721 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.60982 HOMO: -7.15659 LUMO: -0.70205 factor:1 | 1 (-1.82692) | -1 | -1 |
| G: -6257.41721 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.13178 HOMO: -6.69400 LUMO: 1.67622 factor:1 | 1 (-0.34888) | -1 | -1 |
| G: -6257.41721 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.89694 HOMO: -6.60420 LUMO: 2.16058 factor:1 | 1 (-1.11403) | -1 | -1 |
| G: -6257.41721 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.87207 HOMO: -6.87087 LUMO: 1.88031 factor:1 | 1 (-1.08916) | -1 | -1 |
| G: -6257.41721 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.70935 HOMO: -6.60965 LUMO: -0.19864 factor:1 | 1 (-0.92644) | -1 | -1 |
| G: -6257.41721 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.99006 HOMO: -7.29265 LUMO: 0.52246 factor:1 | 1 (-1.20715) | -1 | -1 |
| G: -6257.41721 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.94832 HOMO: -6.86543 LUMO: -0.59593 factor:1 | 1 (-1.16541) | -1 | -1 |
| G: -6257.41721 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.87928 HOMO: -7.44504 LUMO: -1.01226 factor:1 | 1 (-1.09637) | -1 | -1 |
| G: -6257.41721 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.75590 HOMO: -6.92530 LUMO: -0.75103 factor:1 | 1 (-0.97300) | -1 | -1 |
| G: -6257.41721 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.98467 HOMO: -7.10489 LUMO: 2.20412 factor:1 | 1 (-1.20176) | 1 | 1 |
| G: -6257.41721 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.88630 HOMO: -6.58788 LUMO: 1.73881 factor:1 | 1 (-1.10339) | -1 | -1 |
| G: -6257.41721 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.97060 HOMO: -6.64502 LUMO: 1.70343 factor:1 | 1 (-1.18770) | -1 | -1 |
| G: -6257.41721 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.97213 HOMO: -6.73754 LUMO: 1.60819 factor:1 | 1 (-1.18922) | -1 | -1 |
| G: -6257.41721 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.13069 HOMO: -6.80829 LUMO: 2.45991 factor:1 | 1 (-1.34778) | -1 | -1 |
| G: -6257.41721 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.94949 HOMO: -6.91713 LUMO: 2.43814 factor:1 | 1 (-0.16659) | -1 | -1 |
| G: -6257.41721 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.88732 HOMO: -6.60692 LUMO: 1.93745 factor:1 | 1 (-0.10441) | -1 | -1 |
| G: -6257.41721 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.90658 HOMO: -6.26134 LUMO: 1.46125 factor:1 | 1 (-0.12368) | -1 | -1 |
| G: -6257.41721 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.74620 HOMO: -7.54028 LUMO: 0.25851 factor:1 | -1 (0.03671) | -1 | -1 |
| G: -6257.41721 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.11738 HOMO: -6.97700 LUMO: -0.73471 factor:1 | 1 (-1.33447) | -1 | -1 |
| G: -6257.41721 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.19409 HOMO: -6.92258 LUMO: -0.70205 factor:1 | 1 (-1.41118) | -1 | -1 |
| G: -6257.41721 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.10486 HOMO: -6.83550 LUMO: -0.56872 factor:1 | 1 (-1.32196) | -1 | -1 |
| G: -6257.41721 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.85483 HOMO: -6.72121 LUMO: 1.89663 factor:1 | 1 (-0.07192) | -1 | -1 |
| G: -6257.41721 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.91815 HOMO: -6.73482 LUMO: 1.89935 factor:1 | 1 (-0.13524) | -1 | -1 |
| G: -6257.41721 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.72906 HOMO: -6.61781 LUMO: 1.86670 factor:1 | -1 (0.05385) | -1 | -1 |
| G: -6257.41721 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.72800 HOMO: -7.01782 LUMO: 2.26399 factor:1 | 1 (-1.94510) | -1 | -1 |
| G: -6257.41721 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.38343 HOMO: -7.23551 LUMO: 2.09800 factor:1 | 1 (-1.60052) | 1 | 1 |
| G: -6257.41721 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.48264 HOMO: -7.13483 LUMO: 2.17963 factor:1 | 1 (-1.69973) | 1 | 1 |
| G: -6257.41721 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.89912 HOMO: -6.22869 LUMO: 2.01092 factor:1 | 1 (-1.11621) | -1 | -1 |
| G: -6257.41721 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.61325 HOMO: -6.80285 LUMO: 2.14970 factor:1 | 1 (-1.83035) | -1 | -1 |
| G: -6257.41721 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.87384 HOMO: -7.21102 LUMO: 2.33746 factor:1 | 1 (-1.09093) | 1 | 1 |
| G: -6257.41721 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.74733 HOMO: -6.39740 LUMO: 2.59597 factor:1 | 1 (-0.96443) | -1 | -1 |
| G: -6257.41721 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.09597 HOMO: -7.07768 LUMO: 2.48168 factor:1 | 1 (-0.31307) | 1 | 1 |
| G: -6257.41721 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.98612 HOMO: -7.11306 LUMO: 0.90614 factor:1 | 1 (-0.20321) | -1 | -1 |
| G: -6257.41721 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.95616 HOMO: -6.61781 LUMO: -2.46263 factor:1 | 1 (-0.17325) | -1 | -1 |
| G: -6257.41721 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.11720 HOMO: -6.96611 LUMO: 0.90614 factor:1 | 1 (-0.33429) | -1 | -1 |
| G: -6257.41721 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.04441 HOMO: -6.86271 LUMO: -1.14832 factor:1 | 1 (-0.26150) | -1 | -1 |
| G: -6257.41721 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.98501 HOMO: -6.72665 LUMO: 0.96873 factor:1 | 1 (-0.20210) | -1 | -1 |
| G: -6257.41721 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.96228 HOMO: -7.14571 LUMO: 1.05036 factor:1 | 1 (-0.17938) | -1 | -1 |
| G: -6257.41721 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.95798 HOMO: -7.14299 LUMO: 0.98777 factor:1 | 1 (-0.17508) | -1 | -1 |
| G: -6257.41721 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.77390 HOMO: -6.99333 LUMO: 1.05852 factor:1 | -1 (0.00901) | -1 | -1 |
| G: -6257.41721 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.01303 HOMO: -6.78924 LUMO: -1.49935 factor:1 | 1 (-0.23013) | -1 | -1 |
| G: -6257.41721 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.99118 HOMO: -7.13755 LUMO: 0.94151 factor:1 | 1 (-0.20828) | -1 | -1 |
| G: -6257.41721 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.72486 HOMO: -6.72938 LUMO: -0.35375 factor:1 | -1 (0.05804) | -1 | -1 |
| G: -6257.41721 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.79600 HOMO: -6.99061 LUMO: 0.82450 factor:1 | 1 (-0.01309) | -1 | -1 |
| G: -6257.41721 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.16248 HOMO: -6.75114 LUMO: -0.68028 factor:1 | 1 (-0.37957) | -1 | -1 |
| G: -6257.41721 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.05085 HOMO: -6.40556 LUMO: -0.42722 factor:1 | 1 (-1.26794) | -1 | -1 |
| G: -6257.41721 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.58670 HOMO: -7.18653 LUMO: 0.42178 factor:1 | 1 (-1.80379) | -1 | -1 |
| G: -6257.41721 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.88254 HOMO: -6.63958 LUMO: -0.71294 factor:1 | 1 (-2.09963) | -1 | -1 |
| G: -6257.41721 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.42392 HOMO: -6.63958 LUMO: -0.71022 factor:1 | 1 (-1.64101) | -1 | -1 |
| G: -6257.41721 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.31314 HOMO: -6.69672 LUMO: -0.72654 factor:1 | 1 (-1.53023) | -1 | -1 |
| G: -6257.41721 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.65973 HOMO: -6.56883 LUMO: -0.80274 factor:1 | 1 (-1.87682) | -1 | -1 |
| G: -6257.41721 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.68512 HOMO: -6.68584 LUMO: -0.56872 factor:1 | 1 (-1.90221) | -1 | -1 |
| G: -6257.41721 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.68901 HOMO: -6.59060 LUMO: -0.35647 factor:1 | 1 (-1.90610) | -1 | -1 |
| G: -6257.41721 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.00448 HOMO: -6.72121 LUMO: -0.71838 factor:1 | 1 (-1.22157) | -1 | -1 |
| G: -6257.41721 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.97814 HOMO: -6.57971 LUMO: -0.61498 factor:1 | 1 (-1.19523) | -1 | -1 |
| G: -6257.41721 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.96403 HOMO: -7.07496 LUMO: 0.50613 factor:1 | 1 (-0.18112) | -1 | -1 |
| G: -6257.41721 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.91355 HOMO: -7.14027 LUMO: 0.43266 factor:1 | 1 (-0.13064) | -1 | -1 |
| G: -6257.41721 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.04811 HOMO: -6.43277 LUMO: -0.44082 factor:1 | 1 (-0.26520) | -1 | -1 |
| G: -6257.41721 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.06512 HOMO: -6.79468 LUMO: 0.07619 factor:1 | 1 (-0.28221) | -1 | -1 |
| G: -6257.41721 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.83678 HOMO: -6.81917 LUMO: -2.57148 factor:1 | 1 (-1.05387) | -1 | -1 |
| G: -6257.41721 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.62485 HOMO: -6.71849 LUMO: 1.30615 factor:1 | 1 (-0.84195) | -1 | -1 |
| G: -6257.41721 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.91931 HOMO: -6.85455 LUMO: -0.63675 factor:1 | 1 (-1.13640) | -1 | -1 |
| G: -6257.41721 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.87104 HOMO: -6.73210 LUMO: -1.03131 factor:1 | 1 (-1.08813) | -1 | -1 |
| G: -6257.41721 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.83743 HOMO: -6.83550 LUMO: -0.58777 factor:1 | 1 (-1.05452) | -1 | -1 |
| G: -6257.41721 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.89446 HOMO: -6.53073 LUMO: -0.74287 factor:1 | 1 (-1.11156) | -1 | -1 |
| G: -6257.41721 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.90381 HOMO: -7.18381 LUMO: -0.92791 factor:1 | 1 (-0.12090) | -1 | -1 |
| G: -6257.41721 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.64742 HOMO: -6.49264 LUMO: -0.44627 factor:1 | -1 (0.13549) | -1 | -1 |
| G: -6257.41721 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.75458 HOMO: -7.32803 LUMO: 0.41361 factor:1 | -1 (0.02833) | -1 | -1 |
| G: -6257.41721 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.92993 HOMO: -6.53073 LUMO: -0.52790 factor:1 | 1 (-0.14702) | -1 | -1 |
| G: -6257.41721 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.65448 HOMO: -6.54978 LUMO: -0.53062 factor:1 | 1 (-1.87157) | -1 | -1 |
| G: -6257.41721 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.20467 HOMO: -6.56611 LUMO: -0.37824 factor:1 | 1 (-1.42177) | -1 | -1 |
| G: -6257.41721 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.76409 HOMO: -6.57155 LUMO: -0.64219 factor:1 | 1 (-0.98119) | -1 | -1 |
| G: -6257.41721 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.47325 HOMO: -7.08040 LUMO: 0.45715 factor:1 | 1 (-1.69034) | -1 | -1 |
| G: -6257.41721 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.72151 HOMO: -6.66679 LUMO: -0.75376 factor:1 | 1 (-0.93860) | -1 | -1 |
| G: -6257.41721 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.05779 HOMO: -6.83550 LUMO: -0.99322 factor:1 | 1 (-1.27488) | -1 | -1 |
| G: -6257.41721 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.51562 HOMO: -6.53345 LUMO: -0.29660 factor:1 | 1 (-1.73271) | -1 | -1 |
| G: -6257.41721 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.14318 HOMO: -6.65046 LUMO: 2.40549 factor:1 | 1 (-1.36027) | -1 | -1 |
| G: -6257.41721 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.15948 HOMO: -6.98788 LUMO: 2.01092 factor:1 | 1 (-1.37657) | -1 | -1 |
| G: -6257.41721 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.88807 HOMO: -6.61781 LUMO: 1.92384 factor:1 | 1 (-1.10516) | -1 | -1 |
| G: -6257.41721 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.89075 HOMO: -6.61237 LUMO: 2.06807 factor:1 | 1 (-0.10784) | -1 | -1 |
| G: -6257.41721 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.53028 HOMO: -6.59060 LUMO: 1.95106 factor:1 | -1 (0.25263) | -1 | -1 |
| G: -6257.41721 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.44627 HOMO: -6.48175 LUMO: 1.72248 factor:1 | -1 (0.33663) | -1 | -1 |
| G: -6257.41721 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.15560 HOMO: -6.84911 LUMO: 2.03541 factor:1 | -1 (0.62730) | -1 | -1 |
| G: -6257.41721 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.33542 HOMO: -6.50624 LUMO: 2.17147 factor:1 | -1 (0.44749) | -1 | -1 |
| G: -6257.41721 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.44355 HOMO: -6.68312 LUMO: 2.08439 factor:1 | -1 (0.33935) | -1 | -1 |
| G: -6257.41721 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.52435 HOMO: -6.96067 LUMO: 1.98099 factor:1 | 1 (-1.74145) | -1 | -1 |
| G: -6257.41721 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.66604 HOMO: -6.93618 LUMO: 1.85854 factor:1 | 1 (-1.88314) | -1 | -1 |
| G: -6257.41721 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12524.00349 HOMO: -6.71305 LUMO: -0.61226 factor:1 | 1 (-2.22059) | -1 | -1 |
| G: -6257.41721 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.37047 HOMO: -7.06408 LUMO: 0.80001 factor:1 | 1 (-1.58757) | -1 | -1 |
| G: -6257.41721 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.63285 HOMO: -6.52257 LUMO: 0.99049 factor:1 | 1 (-1.84994) | -1 | -1 |
| G: -6257.41721 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.95051 HOMO: -6.84638 LUMO: 1.10750 factor:1 | 1 (-2.16760) | -1 | -1 |
| G: -6257.41721 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.65374 HOMO: -6.85455 LUMO: 0.84900 factor:1 | 1 (-1.87084) | -1 | -1 |
| G: -6257.41721 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.90352 HOMO: -6.60148 LUMO: -0.78369 factor:1 | 1 (-2.12061) | -1 | -1 |
| G: -6257.41721 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12524.26777 HOMO: -6.86543 LUMO: -0.93063 factor:1 | 1 (-2.48486) | -1 | -1 |
| G: -6257.41721 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.39320 HOMO: -6.70489 LUMO: -0.72382 factor:1 | 1 (-0.61030) | -1 | -1 |
| G: -6257.41721 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.47008 HOMO: -6.59060 LUMO: 0.31293 factor:1 | 1 (-0.68717) | -1 | -1 |
| G: -6257.41721 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.97289 HOMO: -6.52257 LUMO: -0.48708 factor:1 | 1 (-1.18998) | -1 | -1 |
| G: -6257.41721 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.05621 HOMO: -6.54706 LUMO: -0.48164 factor:1 | 1 (-1.27330) | -1 | -1 |
| G: -6257.41721 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.49350 HOMO: -7.32803 LUMO: 0.08436 factor:1 | 1 (-0.71060) | -1 | -1 |
| G: -6257.41721 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.36498 HOMO: -6.77291 LUMO: -0.66940 factor:1 | 1 (-1.58207) | -1 | -1 |
| G: -6257.41721 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.99974 HOMO: -6.68312 LUMO: -0.53062 factor:1 | 1 (-2.21683) | -1 | -1 |
| G: -6257.41721 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.51437 HOMO: -7.07768 LUMO: 0.45987 factor:1 | 1 (-1.73146) | -1 | -1 |
| G: -6257.41721 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.95623 HOMO: -6.50352 LUMO: -0.63675 factor:1 | 1 (-2.17332) | -1 | -1 |
| G: -6257.41721 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.62224 HOMO: -6.48992 LUMO: -0.60681 factor:1 | 1 (-0.83934) | -1 | -1 |
| G: -6257.41721 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.45437 HOMO: -6.65318 LUMO: -0.72382 factor:1 | 1 (-0.67147) | -1 | -1 |
| G: -6257.41721 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.46627 HOMO: -6.54706 LUMO: 0.24218 factor:1 | 1 (-0.68336) | -1 | -1 |
| G: -6257.41721 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.74042 HOMO: -6.63958 LUMO: 0.57416 factor:1 | 1 (-0.95751) | -1 | -1 |
| G: -6257.41721 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.26157 HOMO: -6.37563 LUMO: -0.48164 factor:1 | 1 (-1.47867) | -1 | -1 |
| G: -6257.41721 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.18614 HOMO: -6.64774 LUMO: -0.71838 factor:1 | 1 (-1.40324) | -1 | -1 |
| G: -6257.41721 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.17474 HOMO: -7.17020 LUMO: 0.45987 factor:1 | 1 (-1.39184) | -1 | -1 |
| G: -6257.41721 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.58066 HOMO: -6.86543 LUMO: -1.05036 factor:1 | 1 (-0.79776) | -1 | -1 |
| G: -6257.41721 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.31892 HOMO: -6.77019 LUMO: -1.03131 factor:1 | 1 (-0.53601) | -1 | -1 |
| G: -6257.41721 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.46289 HOMO: -6.80285 LUMO: 1.05852 factor:1 | 1 (-0.67999) | -1 | -1 |
| G: -6257.41721 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.05972 HOMO: -6.76475 LUMO: 1.01771 factor:1 | 1 (-1.27681) | -1 | -1 |
| G: -6257.41721 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.94108 HOMO: -6.92530 LUMO: 1.37417 factor:1 | 1 (-1.15817) | -1 | -1 |
| G: -6257.41721 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.19684 HOMO: -6.98244 LUMO: 1.25989 factor:1 | 1 (-1.41393) | -1 | -1 |
| G: -6257.41721 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.65122 HOMO: -6.74842 LUMO: 0.89798 factor:1 | 1 (-0.86832) | -1 | -1 |
| G: -6257.41721 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.48335 HOMO: -6.77019 LUMO: -1.17009 factor:1 | 1 (-0.70045) | -1 | -1 |
| G: -6257.41721 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.27826 HOMO: -6.78652 LUMO: 1.35785 factor:1 | 1 (-0.49536) | -1 | -1 |
| G: -6257.41721 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.01139 HOMO: -6.82734 LUMO: -0.68301 factor:1 | 1 (-1.22849) | -1 | -1 |
| G: -6257.41721 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.79931 HOMO: -6.48175 LUMO: -2.19052 factor:1 | 1 (-1.01640) | -1 | -1 |
| G: -6257.41721 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.12465 HOMO: -6.65863 LUMO: -0.77008 factor:1 | 1 (-1.34174) | -1 | -1 |
| G: -6257.41721 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.29190 HOMO: -6.44094 LUMO: -2.20956 factor:1 | 1 (-0.50899) | -1 | -1 |
| G: -6257.41721 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.54137 HOMO: -6.59876 LUMO: -0.57688 factor:1 | 1 (-0.75846) | -1 | -1 |
| G: -6257.41721 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.70067 HOMO: -6.78380 LUMO: -0.77008 factor:1 | 1 (-0.91776) | -1 | -1 |
| G: -6257.41721 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.72303 HOMO: -7.30354 LUMO: 0.25034 factor:1 | 1 (-0.94013) | -1 | -1 |
| G: -6257.41721 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.23194 HOMO: -6.59332 LUMO: -0.53334 factor:1 | 1 (-1.44903) | -1 | -1 |
| G: -6257.41721 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.61699 HOMO: -6.64230 LUMO: -0.55783 factor:1 | 1 (-0.83408) | -1 | -1 |
| G: -6257.41721 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.10606 HOMO: -7.26544 LUMO: 0.20409 factor:1 | 1 (-1.32315) | -1 | -1 |
| G: -6257.41721 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.22174 HOMO: -6.61237 LUMO: -0.65307 factor:1 | 1 (-1.43883) | -1 | -1 |
| G: -6257.41721 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.65519 HOMO: -6.72393 LUMO: -0.65307 factor:1 | 1 (-0.87229) | -1 | -1 |
| G: -6257.41721 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.65386 HOMO: -6.29671 LUMO: -0.39729 factor:1 | 1 (-0.87095) | -1 | -1 |
| G: -6257.41721 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.74317 HOMO: -6.75387 LUMO: -0.53334 factor:1 | 1 (-0.96026) | -1 | -1 |
| G: -6257.41721 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.26386 HOMO: -6.53073 LUMO: -0.31293 factor:1 | 1 (-1.48095) | -1 | -1 |
| G: -6257.41721 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.22043 HOMO: -6.42189 LUMO: -0.59049 factor:1 | 1 (-1.43752) | -1 | -1 |
| G: -6257.41721 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.33443 HOMO: -6.41100 LUMO: -0.29933 factor:1 | 1 (-0.55152) | -1 | -1 |
| G: -6257.41721 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.48512 HOMO: -6.57427 LUMO: -0.53879 factor:1 | 1 (-0.70222) | -1 | -1 |
| G: -6257.41721 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.54994 HOMO: -7.43143 LUMO: 0.33470 factor:1 | 1 (-0.76703) | -1 | -1 |
| G: -6257.41721 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.24715 HOMO: -6.56067 LUMO: -0.50885 factor:1 | 1 (-1.46424) | -1 | -1 |
| G: -6257.41721 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.07654 HOMO: -6.65863 LUMO: -0.76464 factor:1 | 1 (-1.29363) | -1 | -1 |
| G: -6257.41721 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.92540 HOMO: -6.32665 LUMO: -0.41906 factor:1 | 1 (-1.14250) | -1 | -1 |
| G: -6257.41721 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.67819 HOMO: -6.57699 LUMO: 1.63813 factor:1 | 1 (-0.89528) | -1 | -1 |
| G: -6257.41721 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.02285 HOMO: -6.53073 LUMO: 1.71704 factor:1 | 1 (-1.23994) | -1 | -1 |
| G: -6257.41721 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.11256 HOMO: -6.86271 LUMO: 2.07351 factor:1 | 1 (-1.32966) | -1 | -1 |
| G: -6257.41721 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.64286 HOMO: -6.63686 LUMO: 1.78235 factor:1 | 1 (-1.85995) | -1 | -1 |
| G: -6257.41721 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.62762 HOMO: -6.60965 LUMO: 1.94289 factor:1 | 1 (-1.84471) | -1 | -1 |
| G: -6257.41721 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.05558 HOMO: -6.55250 LUMO: 1.89119 factor:1 | 1 (-1.27268) | -1 | -1 |
| G: -6257.41721 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.07869 HOMO: -6.50624 LUMO: 1.85582 factor:1 | 1 (-1.29578) | -1 | -1 |
| G: -6257.41721 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.52033 HOMO: -6.06814 LUMO: 1.94561 factor:1 | 1 (-1.73742) | -1 | -1 |
| G: -6257.41721 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12524.19005 HOMO: -6.58788 LUMO: 2.01908 factor:1 | 1 (-2.40715) | -1 | -1 |
| G: -6257.41721 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.48707 HOMO: -6.74026 LUMO: 0.31293 factor:1 | 1 (-1.70417) | -1 | -1 |
| G: -6257.41721 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.56308 HOMO: -6.54434 LUMO: -0.42994 factor:1 | 1 (-1.78017) | -1 | -1 |
| G: -6257.41721 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12524.17185 HOMO: -6.94707 LUMO: 0.42994 factor:1 | 1 (-2.38894) | -1 | -1 |
| G: -6257.41721 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12524.04918 HOMO: -6.98516 LUMO: 0.41361 factor:1 | 1 (-2.26627) | -1 | -1 |
| G: -6257.41721 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.55900 HOMO: -6.31304 LUMO: -0.54967 factor:1 | 1 (-0.77610) | -1 | -1 |
| G: -6257.41721 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.13197 HOMO: -6.48447 LUMO: -0.40817 factor:1 | 1 (-1.34906) | -1 | -1 |
| G: -6257.41721 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.10470 HOMO: -6.49264 LUMO: 0.29116 factor:1 | 1 (-1.32179) | -1 | -1 |
| G: -6257.41721 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.06100 HOMO: -6.48719 LUMO: -0.11973 factor:1 | 1 (-1.27809) | -1 | -1 |
| G: -6257.41721 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.50991 HOMO: -7.16204 LUMO: 0.44082 factor:1 | 1 (-0.72701) | -1 | -1 |
| G: -6257.41721 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.07139 HOMO: -6.74842 LUMO: -0.37552 factor:1 | 1 (-1.28849) | -1 | -1 |
| G: -6257.41721 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.54172 HOMO: -6.44638 LUMO: -0.45171 factor:1 | 1 (-0.75882) | -1 | -1 |
| G: -6257.41721 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.04960 HOMO: -7.07496 LUMO: 0.50341 factor:1 | 1 (-1.26669) | -1 | -1 |
| G: -6257.41721 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.86369 HOMO: -6.79468 LUMO: 0.11429 factor:1 | 1 (-1.08078) | -1 | -1 |
| G: -6257.41721 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.11648 HOMO: -6.63958 LUMO: -0.67484 factor:1 | 1 (-1.33358) | -1 | -1 |
| G: -6257.41721 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.45508 HOMO: -7.08584 LUMO: 0.46259 factor:1 | 1 (-0.67218) | -1 | -1 |
| G: -6257.41721 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.08380 HOMO: -6.80285 LUMO: -0.73199 factor:1 | 1 (-1.30089) | -1 | -1 |
| G: -6257.41721 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.02679 HOMO: -6.44366 LUMO: -0.45443 factor:1 | 1 (-1.24389) | -1 | -1 |
| G: -6257.41721 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.92627 HOMO: -6.75931 LUMO: 0.25851 factor:1 | 1 (-1.14337) | -1 | -1 |
| G: -6257.41721 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.47625 HOMO: -6.64502 LUMO: 1.79323 factor:1 | 1 (-0.69335) | -1 | -1 |
| G: -6257.41721 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.35143 HOMO: -6.51168 LUMO: 1.60275 factor:1 | 1 (-0.56853) | -1 | -1 |
| G: -6257.41721 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.21042 HOMO: -6.56067 LUMO: 1.63268 factor:1 | 1 (-1.42751) | -1 | -1 |
| G: -6257.41721 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.57801 HOMO: -6.56883 LUMO: 1.70615 factor:1 | 1 (-1.79511) | -1 | -1 |
| G: -6257.41721 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12524.37974 HOMO: -6.77836 LUMO: 1.77962 factor:1 | 1 (-2.59684) | -1 | -1 |
| G: -6257.41721 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12524.37958 HOMO: -6.38923 LUMO: 1.85854 factor:1 | 1 (-2.59667) | -1 | -1 |
| G: -6257.41721 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12524.38793 HOMO: -6.35658 LUMO: 2.16875 factor:1 | 1 (-2.60503) | -1 | -1 |
| G: -6257.41721 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.06073 HOMO: -6.83006 LUMO: 2.31025 factor:1 | 1 (-1.27782) | -1 | -1 |
| G: -6257.41721 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.99844 HOMO: -6.87087 LUMO: 1.79051 factor:1 | 1 (-1.21553) | -1 | -1 |
| G: -6257.41721 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.65506 HOMO: -6.56339 LUMO: 2.37828 factor:1 | 1 (-0.87215) | -1 | -1 |
| G: -6257.41721 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.44858 HOMO: -6.30488 LUMO: 2.51705 factor:1 | 1 (-0.66567) | -1 | -1 |
| G: -6257.41721 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.17725 HOMO: -6.69400 LUMO: 1.95650 factor:1 | 1 (-0.39435) | -1 | -1 |
| G: -6257.41721 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.06894 HOMO: -6.51168 LUMO: 2.03541 factor:1 | 1 (-1.28604) | -1 | -1 |
| G: -6257.41721 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.99446 HOMO: -6.30760 LUMO: 1.65173 factor:1 | 1 (-2.21155) | -1 | -1 |
| G: -6257.41721 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.04992 HOMO: -6.55250 LUMO: 1.90752 factor:1 | 1 (-1.26702) | -1 | -1 |
| G: -6257.41721 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12524.06962 HOMO: -6.41372 LUMO: 1.76058 factor:1 | 1 (-2.28671) | -1 | -1 |
| G: -6257.41721 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.98480 HOMO: -6.23957 LUMO: 2.06534 factor:1 | 1 (-2.20189) | -1 | -1 |
| G: -6257.41721 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.42789 HOMO: -6.58243 LUMO: 2.11705 factor:1 | 1 (-1.64498) | -1 | -1 |
| G: -6257.41721 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.68814 HOMO: -6.37835 LUMO: 2.09256 factor:1 | 1 (-1.90523) | -1 | -1 |
| G: -6257.41721 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.34713 HOMO: -6.50624 LUMO: 2.55787 factor:1 | 1 (-1.56422) | -1 | -1 |
| G: -6257.41721 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.42472 HOMO: -6.45454 LUMO: 1.87214 factor:1 | -1 (0.35818) | -1 | -1 |
| G: -6257.41721 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.03771 HOMO: -6.53617 LUMO: 1.95650 factor:1 | 1 (-1.25480) | -1 | -1 |
| G: -6257.41721 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.13088 HOMO: -6.51985 LUMO: 1.71432 factor:1 | 1 (-1.34797) | -1 | -1 |
| G: -6257.41721 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.81523 HOMO: -6.75114 LUMO: 1.84493 factor:1 | 1 (-1.03232) | -1 | -1 |
| G: -6257.41721 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.32801 HOMO: -6.06270 LUMO: 1.65717 factor:1 | -1 (0.45489) | -1 | -1 |
| G: -6257.41721 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.29926 HOMO: -5.89671 LUMO: 1.71704 factor:1 | 1 (-1.51635) | -1 | -1 |
| G: -6257.41721 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.39894 HOMO: -6.18787 LUMO: 1.91840 factor:1 | 1 (-1.61603) | -1 | -1 |
| G: -6257.41721 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.07025 HOMO: -6.01644 LUMO: 1.85582 factor:1 | 1 (-1.28734) | -1 | -1 |
| G: -6257.41721 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.94582 HOMO: -6.05998 LUMO: 2.33474 factor:1 | 1 (-0.16291) | -1 | -1 |
| G: -6257.41721 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.06520 HOMO: -6.05725 LUMO: 2.03541 factor:1 | 1 (-0.28229) | -1 | -1 |
| G: -6257.41721 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.74008 HOMO: -6.80829 LUMO: 1.90480 factor:1 | -1 (0.04283) | -1 | -1 |
| G: -6257.41721 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.30678 HOMO: -6.76475 LUMO: 2.20956 factor:1 | 1 (-0.52387) | -1 | -1 |
| G: -6257.41721 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.67126 HOMO: -6.29944 LUMO: 1.77962 factor:1 | -1 (0.11165) | -1 | -1 |
| G: -6257.41721 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.35280 HOMO: -6.47359 LUMO: -0.25579 factor:1 | -1 (0.43010) | -1 | -1 |
| G: -6257.41721 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.05504 HOMO: -6.57699 LUMO: -0.47348 factor:1 | 1 (-1.27213) | -1 | -1 |
| G: -6257.41721 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.61053 HOMO: -7.20830 LUMO: 0.49797 factor:1 | 1 (-1.82763) | -1 | -1 |
| G: -6257.41721 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.10748 HOMO: -7.49402 LUMO: 0.29933 factor:1 | 1 (-1.32457) | -1 | -1 |
| G: -6257.41721 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.76423 HOMO: -6.66679 LUMO: -0.58777 factor:1 | 1 (-0.98132) | -1 | -1 |
| G: -6257.41721 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.55330 HOMO: -6.67767 LUMO: -0.56328 factor:1 | -1 (0.22961) | -1 | -1 |
| G: -6257.41721 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.49230 HOMO: -7.42871 LUMO: 0.35647 factor:1 | 1 (-1.70939) | -1 | -1 |
| G: -6257.41721 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.65282 HOMO: -6.56067 LUMO: -0.54423 factor:1 | 1 (-1.86991) | -1 | -1 |
| G: -6257.41721 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.24244 HOMO: -6.56339 LUMO: -0.50341 factor:1 | 1 (-1.45954) | -1 | -1 |
| G: -6257.41721 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.15268 HOMO: -6.56067 LUMO: -0.48436 factor:1 | 1 (-0.36978) | -1 | -1 |
| G: -6257.41721 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.35293 HOMO: -6.73210 LUMO: 1.75241 factor:1 | 1 (-0.57002) | -1 | -1 |
| G: -6257.41721 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.98397 HOMO: -6.48175 LUMO: 1.91296 factor:1 | 1 (-0.20106) | -1 | -1 |
| G: -6257.41721 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.68306 HOMO: -6.67767 LUMO: 1.70343 factor:1 | 1 (-0.90015) | -1 | -1 |
| G: -6257.41721 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.25768 HOMO: -6.37835 LUMO: 1.96466 factor:1 | 1 (-1.47478) | -1 | -1 |
| G: -6257.41721 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.45499 HOMO: -6.40828 LUMO: 2.10072 factor:1 | 1 (-1.67209) | -1 | -1 |
| G: -6257.41721 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.08448 HOMO: -6.06542 LUMO: 1.92112 factor:1 | 1 (-1.30158) | -1 | -1 |
| G: -6257.41721 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.16880 HOMO: -6.90353 LUMO: 1.83133 factor:1 | -1 (0.61411) | -1 | -1 |
| G: -6257.41721 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.62416 HOMO: -6.37019 LUMO: 1.92929 factor:1 | -1 (0.15875) | -1 | -1 |
| G: -6257.41721 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.45003 HOMO: -6.61509 LUMO: 2.11160 factor:1 | -1 (0.33288) | -1 | -1 |
| G: -6257.41721 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.85411 HOMO: -6.82734 LUMO: 1.77146 factor:1 | 1 (-1.07120) | -1 | -1 |
| G: -6257.41721 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.07681 HOMO: -6.01100 LUMO: 1.89935 factor:1 | 1 (-1.29390) | -1 | -1 |
| G: -6257.41721 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.81631 HOMO: -6.49536 LUMO: 1.75241 factor:1 | 1 (-1.03341) | -1 | -1 |
| G: -6257.41721 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.03663 HOMO: -6.34297 LUMO: 1.86398 factor:1 | -1 (0.74627) | -1 | -1 |
| G: -6257.41721 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.19500 HOMO: -6.53073 LUMO: 1.84493 factor:1 | -1 (0.58790) | -1 | -1 |
| G: -6257.41721 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.11238 HOMO: -6.53345 LUMO: 2.41093 factor:1 | 1 (-0.32948) | -1 | -1 |
| G: -6257.41721 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.29979 HOMO: -7.01237 LUMO: 2.06262 factor:1 | 1 (-0.51688) | -1 | -1 |
| G: -6257.41721 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.93028 HOMO: -6.17154 LUMO: 1.89119 factor:1 | 1 (-0.14738) | -1 | -1 |
| G: -6257.41721 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.42235 HOMO: -6.08719 LUMO: 1.74425 factor:1 | 1 (-0.63944) | -1 | -1 |
| G: -6257.41721 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12520.46637 HOMO: -6.69672 LUMO: 1.95106 factor:1 | -1 (1.31654) | -1 | -1 |
| G: -6257.41721 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.05767 HOMO: -6.58243 LUMO: 2.24766 factor:1 | -1 (0.72524) | -1 | -1 |
| G: -6257.41721 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12520.91318 HOMO: -6.74570 LUMO: 2.02181 factor:1 | -1 (0.86973) | -1 | -1 |
| G: -6257.41721 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.23150 HOMO: -6.53890 LUMO: 1.92929 factor:1 | -1 (0.55141) | -1 | -1 |
| G: -6257.41721 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.30673 HOMO: -6.03276 LUMO: 1.67078 factor:1 | 1 (-0.52382) | -1 | -1 |
| G: -6257.41721 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12520.14056 HOMO: -6.67767 LUMO: 2.03541 factor:1 | -1 (1.64234) | -1 | -1 |
| G: -6257.41721 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12520.90485 HOMO: -5.98378 LUMO: 1.84221 factor:1 | -1 (0.87806) | -1 | -1 |
| G: -6257.41721 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.37099 HOMO: -6.07086 LUMO: 2.01908 factor:1 | 1 (-1.58808) | -1 | -1 |
| G: -6257.41721 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.54522 HOMO: -6.29944 LUMO: 1.90208 factor:1 | 1 (-1.76232) | -1 | -1 |
| G: -6257.41721 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.20625 HOMO: -6.75114 LUMO: 1.85854 factor:1 | 1 (-1.42335) | -1 | -1 |
| G: -6257.41721 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.59751 HOMO: -6.56611 LUMO: 2.49801 factor:1 | 1 (-0.81460) | -1 | -1 |
| G: -6257.41721 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.01099 HOMO: -6.39740 LUMO: 1.92929 factor:1 | 1 (-0.22809) | -1 | -1 |
| G: -6257.41721 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.14792 HOMO: -6.85999 LUMO: -1.07757 factor:1 | 1 (-0.36501) | -1 | -1 |
| G: -6257.41721 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.86274 HOMO: -6.98244 LUMO: 1.07213 factor:1 | 1 (-0.07984) | -1 | -1 |
| G: -6257.41721 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.25772 HOMO: -7.04231 LUMO: 0.64219 factor:1 | 1 (-0.47481) | -1 | -1 |
| G: -6257.41721 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.03201 HOMO: -6.96339 LUMO: 0.75648 factor:1 | -1 (0.75090) | -1 | -1 |
| G: -6257.41721 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12520.97563 HOMO: -6.83822 LUMO: -0.97417 factor:1 | -1 (0.80728) | -1 | -1 |
| G: -6257.41721 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.22633 HOMO: -6.44910 LUMO: -2.15242 factor:1 | 1 (-1.44343) | -1 | -1 |
| G: -6257.41721 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.33554 HOMO: -6.84094 LUMO: -1.37690 factor:1 | 1 (-0.55264) | -1 | -1 |
| G: -6257.41721 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.39992 HOMO: -6.74026 LUMO: -2.54699 factor:1 | 1 (-1.61701) | -1 | -1 |
| G: -6257.41721 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.46159 HOMO: -6.96611 LUMO: 1.24900 factor:1 | 1 (-0.67868) | -1 | -1 |
| G: -6257.41721 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.10089 HOMO: -7.21102 LUMO: 0.82995 factor:1 | 1 (-1.31798) | -1 | -1 |
| G: -6257.41721 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.18751 HOMO: -6.88448 LUMO: 0.81634 factor:1 | 1 (-0.40461) | -1 | -1 |
| G: -6257.41721 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.64349 HOMO: -7.04231 LUMO: 1.10750 factor:1 | 1 (-0.86059) | -1 | -1 |
| G: -6257.41721 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.34156 HOMO: -6.83550 LUMO: -0.98777 factor:1 | 1 (-0.55865) | -1 | -1 |
| G: -6257.41721 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.10810 HOMO: -6.82189 LUMO: 0.93879 factor:1 | 1 (-1.32519) | -1 | -1 |
| G: -6257.41721 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.87647 HOMO: -6.81101 LUMO: 0.70750 factor:1 | 1 (-2.09356) | -1 | -1 |
| G: -6257.41721 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.23091 HOMO: -7.06680 LUMO: 0.74015 factor:1 | 1 (-1.44800) | -1 | -1 |
| G: -6257.41721 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.97920 HOMO: -6.68856 LUMO: 0.86260 factor:1 | 1 (-1.19629) | -1 | -1 |
| G: -6257.41721 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.20281 HOMO: -6.83822 LUMO: -0.63403 factor:1 | -1 (0.58009) | -1 | -1 |
| G: -6257.41721 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.03672 HOMO: -6.84911 LUMO: 1.26533 factor:1 | -1 (0.74619) | -1 | -1 |
| G: -6257.41721 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.34833 HOMO: -7.01237 LUMO: 0.73743 factor:1 | 1 (-0.56543) | -1 | -1 |
| G: -6257.41721 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.00824 HOMO: -7.00965 LUMO: 1.40139 factor:1 | 1 (-0.22534) | -1 | -1 |
| G: -6257.41721 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12520.72349 HOMO: -6.73210 LUMO: -2.49256 factor:1 | -1 (1.05942) | -1 | -1 |
| G: -6257.41721 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12520.86183 HOMO: -7.08040 LUMO: 0.84627 factor:1 | -1 (0.92108) | -1 | -1 |
| G: -6257.41721 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.33374 HOMO: -7.00965 LUMO: 0.82995 factor:1 | 1 (-1.55083) | -1 | -1 |
| G: -6257.41721 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.07267 HOMO: -6.88448 LUMO: 0.82723 factor:1 | 1 (-1.28977) | -1 | -1 |
| G: -6257.41721 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.37036 HOMO: -7.20013 LUMO: 0.88437 factor:1 | 1 (-1.58746) | -1 | -1 |
| G: -6257.41721 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.91688 HOMO: -6.60420 LUMO: -0.53334 factor:1 | 1 (-2.13397) | -1 | -1 |
| G: -6257.41721 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.89904 HOMO: -6.78652 LUMO: -0.79729 factor:1 | 1 (-1.11613) | -1 | -1 |
| G: -6257.41721 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.13499 HOMO: -6.48992 LUMO: -0.64491 factor:1 | 1 (-1.35208) | -1 | -1 |
| G: -6257.41721 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.73158 HOMO: -6.85999 LUMO: -0.78097 factor:1 | 1 (-0.94867) | -1 | -1 |
| G: -6257.41721 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.10204 HOMO: -6.65046 LUMO: -0.78097 factor:1 | 1 (-0.31914) | -1 | -1 |
| G: -6257.41721 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.88212 HOMO: -7.24095 LUMO: 0.37280 factor:1 | 1 (-0.09921) | -1 | -1 |
| G: -6257.41721 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.93741 HOMO: -6.81101 LUMO: -0.74831 factor:1 | 1 (-0.15451) | -1 | -1 |
| G: -6257.41721 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.20558 HOMO: -6.69400 LUMO: -0.77280 factor:1 | 1 (-0.42267) | -1 | -1 |
| G: -6257.41721 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.03282 HOMO: -6.08447 LUMO: -0.68573 factor:1 | 1 (-0.24991) | -1 | -1 |
| G: -6257.41721 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.77001 HOMO: -6.66679 LUMO: -0.47076 factor:1 | -1 (0.01290) | -1 | -1 |
| G: -6257.41721 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.80114 HOMO: -6.97428 LUMO: -1.10750 factor:1 | 1 (-0.01823) | -1 | -1 |
| G: -6257.41721 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.12433 HOMO: -6.69128 LUMO: -0.54151 factor:1 | 1 (-0.34142) | -1 | -1 |
| G: -6257.41721 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.78881 HOMO: -6.53617 LUMO: -0.35375 factor:1 | 1 (-0.00590) | -1 | -1 |
| G: -6257.41721 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.69504 HOMO: -6.75659 LUMO: -0.41361 factor:1 | -1 (0.08787) | -1 | -1 |
| G: -6257.41721 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.02789 HOMO: -6.69400 LUMO: -0.67484 factor:1 | 1 (-0.24498) | -1 | -1 |
| G: -6257.41721 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.90601 HOMO: -6.89264 LUMO: -0.90886 factor:1 | 1 (-0.12310) | -1 | -1 |
| G: -6257.41721 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.38239 HOMO: -6.56339 LUMO: -0.52518 factor:1 | 1 (-1.59949) | -1 | -1 |
| G: -6257.41721 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12524.12173 HOMO: -6.45726 LUMO: -0.65852 factor:1 | 1 (-2.33882) | -1 | -1 |
| G: -6257.41721 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.18598 HOMO: -6.80557 LUMO: -0.56600 factor:1 | 1 (-1.40307) | -1 | -1 |
| G: -6257.41721 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.87199 HOMO: -7.19469 LUMO: -0.91702 factor:1 | 1 (-1.08908) | -1 | -1 |
| G: -6257.41721 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.68464 HOMO: -6.41100 LUMO: 0.79185 factor:1 | 1 (-0.90173) | -1 | -1 |
| G: -6257.41721 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12520.91944 HOMO: -6.39195 LUMO: 0.26123 factor:1 | -1 (0.86347) | -1 | -1 |
| G: -6257.41721 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.10888 HOMO: -6.78924 LUMO: 0.35919 factor:1 | -1 (0.67403) | -1 | -1 |
| G: -6257.41721 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.05801 HOMO: -6.50624 LUMO: 0.71838 factor:1 | 1 (-1.27510) | -1 | -1 |
| G: -6257.41721 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.84554 HOMO: -6.68584 LUMO: -0.66124 factor:1 | 1 (-1.06263) | -1 | -1 |
| G: -6257.41721 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12520.99451 HOMO: -6.45182 LUMO: -0.48980 factor:1 | -1 (0.78840) | -1 | -1 |
| G: -6257.41721 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.11854 HOMO: -7.18925 LUMO: -1.01498 factor:1 | -1 (0.66437) | -1 | -1 |
| G: -6257.41721 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12520.96888 HOMO: -7.18925 LUMO: -0.63130 factor:1 | -1 (0.81403) | -1 | -1 |
| G: -6257.41721 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.80683 HOMO: -6.66679 LUMO: -0.57960 factor:1 | 1 (-0.02392) | -1 | -1 |
| G: -6257.41721 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.96079 HOMO: -6.44910 LUMO: -0.30205 factor:1 | 1 (-0.17788) | -1 | -1 |
| G: -6257.41721 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.85243 HOMO: -7.23279 LUMO: 0.46804 factor:1 | 1 (-0.06953) | -1 | -1 |
| G: -6257.41721 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.40030 HOMO: -6.92802 LUMO: -0.72927 factor:1 | 1 (-1.61739) | -1 | -1 |
| G: -6257.41721 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.88844 HOMO: -6.83278 LUMO: -0.59321 factor:1 | 1 (-2.10554) | -1 | -1 |
| G: -6257.41721 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.04258 HOMO: -7.44776 LUMO: 0.27211 factor:1 | 1 (-1.25967) | -1 | -1 |
| G: -6257.41721 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.63416 HOMO: -6.80829 LUMO: -0.59865 factor:1 | 1 (-0.85125) | -1 | -1 |
| G: -6257.41721 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.79069 HOMO: -6.63686 LUMO: -0.75103 factor:1 | 1 (-0.00778) | -1 | -1 |
| G: -6257.41721 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.05736 HOMO: -6.73210 LUMO: -0.55511 factor:1 | 1 (-0.27445) | -1 | -1 |
| G: -6257.41721 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.71506 HOMO: -6.50624 LUMO: 1.58642 factor:1 | 1 (-0.93215) | -1 | -1 |
| G: -6257.41721 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.66134 HOMO: -6.79196 LUMO: 0.96328 factor:1 | 1 (-1.87843) | -1 | -1 |
| G: -6257.41721 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.74877 HOMO: -6.82734 LUMO: 1.23540 factor:1 | 1 (-0.96587) | -1 | -1 |
| G: -6257.41721 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.00562 HOMO: -6.90081 LUMO: 1.25444 factor:1 | 1 (-1.22272) | -1 | -1 |
| G: -6257.41721 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.54778 HOMO: -7.00965 LUMO: -1.05036 factor:1 | 1 (-1.76488) | -1 | -1 |
| G: -6257.41721 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.83193 HOMO: -7.01237 LUMO: -1.48302 factor:1 | 1 (-1.04903) | -1 | -1 |
| G: -6257.41721 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.79152 HOMO: -6.91713 LUMO: 0.93607 factor:1 | 1 (-1.00862) | -1 | -1 |
| G: -6257.41721 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.97218 HOMO: -7.02598 LUMO: 0.92247 factor:1 | 1 (-1.18927) | -1 | -1 |
| G: -6257.41721 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.19140 HOMO: -6.98516 LUMO: 1.52384 factor:1 | 1 (-0.40850) | -1 | -1 |
| G: -6257.41721 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.35192 HOMO: -6.75387 LUMO: 1.04764 factor:1 | 1 (-0.56902) | -1 | -1 |
| G: -6257.41721 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.27606 HOMO: -7.09401 LUMO: 1.19458 factor:1 | 1 (-0.49315) | -1 | -1 |
| G: -6257.41721 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.96805 HOMO: -6.88992 LUMO: -1.56193 factor:1 | 1 (-0.18515) | -1 | -1 |
| G: -6257.41721 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.63879 HOMO: -7.00149 LUMO: 0.99866 factor:1 | 1 (-0.85588) | -1 | -1 |
| G: -6257.41721 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.73667 HOMO: -7.13755 LUMO: 1.05308 factor:1 | 1 (-0.95376) | -1 | -1 |
| G: -6257.41721 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.50237 HOMO: -6.85183 LUMO: -1.42860 factor:1 | 1 (-1.71946) | -1 | -1 |
| G: -6257.41721 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.52520 HOMO: -6.63141 LUMO: -0.88981 factor:1 | 1 (-1.74229) | -1 | -1 |
| G: -6257.41721 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.68986 HOMO: -6.92258 LUMO: -0.82178 factor:1 | 1 (-0.90696) | -1 | -1 |
| G: -6257.41721 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.24946 HOMO: -6.55794 LUMO: -0.80818 factor:1 | 1 (-1.46656) | -1 | -1 |
| G: -6257.41721 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.43285 HOMO: -6.95251 LUMO: -0.97145 factor:1 | 1 (-0.64994) | -1 | -1 |
| G: -6257.41721 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.22722 HOMO: -7.37701 LUMO: 0.14150 factor:1 | -1 (0.55568) | -1 | -1 |
| G: -6257.41721 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.32290 HOMO: -6.74842 LUMO: -0.68028 factor:1 | -1 (0.46001) | -1 | -1 |
| G: -6257.41721 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12520.74735 HOMO: -6.65046 LUMO: -0.52518 factor:1 | -1 (1.03556) | -1 | -1 |
| G: -6257.41721 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12520.95089 HOMO: -6.91441 LUMO: -1.13199 factor:1 | -1 (0.83202) | -1 | -1 |
| G: -6257.41721 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12520.15899 HOMO: -7.00965 LUMO: -1.00682 factor:1 | -1 (1.62392) | -1 | -1 |
| G: -6257.41721 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12520.46275 HOMO: -6.55794 LUMO: -0.54967 factor:1 | -1 (1.32016) | -1 | -1 |
| G: -6257.41721 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12520.58041 HOMO: -6.71577 LUMO: -0.53879 factor:1 | -1 (1.20250) | -1 | -1 |
| G: -6257.41721 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12519.95817 HOMO: -6.88992 LUMO: -0.55511 factor:1 | -1 (1.82474) | -1 | -1 |
| G: -6257.41721 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12520.76474 HOMO: -6.74026 LUMO: -0.60681 factor:1 | -1 (1.01817) | -1 | -1 |
| G: -6257.41721 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.69033 HOMO: -6.76747 LUMO: -0.50885 factor:1 | -1 (0.09257) | -1 | -1 |
| G: -6257.41721 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.52715 HOMO: -6.87904 LUMO: -0.92519 factor:1 | -1 (0.25576) | -1 | -1 |
| G: -6257.41721 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.22268 HOMO: -6.53073 LUMO: -0.53062 factor:1 | -1 (0.56023) | -1 | -1 |
| G: -6257.41721 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.25642 HOMO: -6.97700 LUMO: -0.98505 factor:1 | -1 (0.52649) | -1 | -1 |
| G: -6257.41721 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.36867 HOMO: -6.96884 LUMO: -0.79185 factor:1 | -1 (0.41424) | -1 | -1 |
| G: -6257.41721 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.06727 HOMO: -6.60420 LUMO: -0.31021 factor:1 | -1 (0.71563) | -1 | -1 |
| G: -6257.41721 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.41313 HOMO: -6.68584 LUMO: -0.63947 factor:1 | -1 (0.36978) | -1 | -1 |
| G: -6257.41721 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12520.91459 HOMO: -6.41917 LUMO: -0.35103 factor:1 | -1 (0.86832) | -1 | -1 |
| G: -6257.41721 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.12621 HOMO: -6.73482 LUMO: -0.70477 factor:1 | -1 (0.65669) | -1 | -1 |
| G: -6257.41721 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.24186 HOMO: -6.71305 LUMO: -0.85716 factor:1 | -1 (0.54104) | -1 | -1 |
| G: -6257.41721 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.04869 HOMO: -6.70761 LUMO: -0.63403 factor:1 | -1 (0.73422) | -1 | -1 |
| G: -6257.41721 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12520.78368 HOMO: -6.37563 LUMO: -0.38640 factor:1 | -1 (0.99923) | -1 | -1 |
| G: -6257.41721 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.34143 HOMO: -6.27495 LUMO: -0.54967 factor:1 | -1 (0.44148) | -1 | -1 |
| G: -6257.41721 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.65409 HOMO: -6.98516 LUMO: 0.38096 factor:1 | -1 (0.12882) | -1 | -1 |
| G: -6257.41721 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.75327 HOMO: -6.47087 LUMO: -0.40001 factor:1 | -1 (0.02963) | -1 | -1 |
| G: -6257.41721 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.39299 HOMO: -6.59876 LUMO: 0.20681 factor:1 | -1 (0.38991) | -1 | -1 |
| G: -6257.41721 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.78699 HOMO: -6.89809 LUMO: 0.14966 factor:1 | 1 (-0.00408) | -1 | -1 |
| G: -6257.41721 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.91513 HOMO: -6.76203 LUMO: 2.11432 factor:1 | 1 (-0.13222) | -1 | -1 |
| G: -6257.41721 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.48183 HOMO: -6.58516 LUMO: 1.75786 factor:1 | 1 (-0.69892) | -1 | -1 |
| G: -6257.41721 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.57239 HOMO: -6.37835 LUMO: 1.84493 factor:1 | 1 (-0.78948) | -1 | -1 |
| G: -6257.41721 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.75835 HOMO: -6.83550 LUMO: 1.74425 factor:1 | 1 (-0.97545) | -1 | -1 |
| G: -6257.41721 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.58996 HOMO: -6.65318 LUMO: 1.79051 factor:1 | 1 (-1.80705) | -1 | -1 |
| G: -6257.41721 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.53565 HOMO: -6.68584 LUMO: 2.11160 factor:1 | 1 (-1.75274) | -1 | -1 |
| G: -6257.41721 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.69680 HOMO: -6.36202 LUMO: 1.85037 factor:1 | 1 (-0.91389) | -1 | -1 |
| G: -6257.41721 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.41922 HOMO: -6.68312 LUMO: 2.23133 factor:1 | 1 (-0.63631) | -1 | -1 |
| G: -6257.41721 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.53179 HOMO: -6.66679 LUMO: 2.14154 factor:1 | 1 (-0.74888) | -1 | -1 |
| G: -6257.41721 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.75865 HOMO: -6.50896 LUMO: 1.92657 factor:1 | 1 (-0.97575) | -1 | -1 |
| G: -6257.41721 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.73710 HOMO: -6.63686 LUMO: 2.22317 factor:1 | 1 (-0.95419) | -1 | -1 |
| G: -6257.41721 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.61745 HOMO: -6.58788 LUMO: 2.17419 factor:1 | 1 (-0.83455) | -1 | -1 |
| G: -6257.41721 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.30879 HOMO: -6.72665 LUMO: 2.12249 factor:1 | 1 (-0.52589) | -1 | -1 |
| G: -6257.41721 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.53174 HOMO: -6.28311 LUMO: 1.91024 factor:1 | 1 (-0.74883) | -1 | -1 |
| G: -6257.41721 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.37905 HOMO: -6.56067 LUMO: 2.27487 factor:1 | 1 (-0.59615) | -1 | -1 |
| G: -6257.41721 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.42733 HOMO: -6.83006 LUMO: 2.28031 factor:1 | 1 (-0.64442) | -1 | -1 |
| G: -6257.41721 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.31301 HOMO: -6.45182 LUMO: 1.62724 factor:1 | 1 (-0.53011) | -1 | -1 |
| G: -6257.41721 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.30907 HOMO: -6.78380 LUMO: 1.83677 factor:1 | 1 (-0.52616) | -1 | -1 |
| G: -6257.41721 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.40817 HOMO: -6.23413 LUMO: 1.80956 factor:1 | 1 (-0.62526) | -1 | -1 |
| G: -6257.41721 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.54755 HOMO: -6.74298 LUMO: 2.16875 factor:1 | 1 (-0.76464) | -1 | -1 |
| G: -6257.41721 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.20281 HOMO: -6.81645 LUMO: 2.50073 factor:1 | 1 (-0.41990) | -1 | -1 |
| G: -6257.41721 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.34948 HOMO: -6.71033 LUMO: 1.96466 factor:1 | -1 (0.43342) | -1 | -1 |
| G: -6257.41721 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.12768 HOMO: -6.83550 LUMO: 2.04358 factor:1 | -1 (0.65522) | -1 | -1 |
| G: -6257.41721 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.12474 HOMO: -6.60965 LUMO: 2.38100 factor:1 | -1 (0.65816) | -1 | -1 |
| G: -6257.41721 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.83395 HOMO: -6.73210 LUMO: 2.26127 factor:1 | 1 (-1.05104) | -1 | -1 |
| G: -6257.41721 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.58820 HOMO: -6.76203 LUMO: 2.13609 factor:1 | 1 (-0.80529) | -1 | -1 |
| G: -6257.41721 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.28184 HOMO: -6.71033 LUMO: 2.05990 factor:1 | -1 (0.50107) | -1 | -1 |
| G: -6257.41721 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.26004 HOMO: -6.50896 LUMO: 2.32385 factor:1 | -1 (0.52287) | -1 | -1 |
| G: -6257.41721 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.68183 HOMO: -6.53345 LUMO: 1.74425 factor:1 | 1 (-0.89893) | -1 | -1 |
| G: -6257.41721 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.30994 HOMO: -6.25862 LUMO: 1.63540 factor:1 | 1 (-0.52703) | -1 | -1 |
| G: -6257.41721 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.76053 HOMO: -5.90759 LUMO: 1.78779 factor:1 | 1 (-0.97762) | -1 | -1 |
| G: -6257.41721 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.42861 HOMO: -6.09807 LUMO: 1.99732 factor:1 | 1 (-0.64570) | -1 | -1 |
| G: -6257.41721 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.18885 HOMO: -5.92392 LUMO: 1.99732 factor:1 | 1 (-0.40594) | -1 | -1 |
| G: -6257.41721 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.50170 HOMO: -6.45182 LUMO: 1.72248 factor:1 | -1 (0.28120) | -1 | -1 |
| G: -6257.41721 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.36208 HOMO: -6.53073 LUMO: 1.82588 factor:1 | -1 (0.42082) | -1 | -1 |
| G: -6257.41721 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.47719 HOMO: -6.40828 LUMO: 2.05174 factor:1 | -1 (0.30572) | -1 | -1 |
| G: -6257.41721 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.14836 HOMO: -6.60420 LUMO: -0.82450 factor:1 | -1 (0.63454) | -1 | -1 |
| G: -6257.41721 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.27950 HOMO: -6.76747 LUMO: -0.57144 factor:1 | -1 (0.50341) | -1 | -1 |
| G: -6257.41721 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.20603 HOMO: -6.67767 LUMO: -0.59321 factor:1 | -1 (0.57688) | -1 | -1 |
| G: -6257.41721 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.41621 HOMO: -6.65863 LUMO: -0.57416 factor:1 | -1 (0.36670) | -1 | -1 |
| G: -6257.41721 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.47961 HOMO: -6.49808 LUMO: -0.54695 factor:1 | -1 (0.30330) | -1 | -1 |
| G: -6257.41721 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.72666 HOMO: -6.50080 LUMO: -0.61498 factor:1 | -1 (0.05625) | -1 | -1 |
| G: -6257.41721 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.01263 HOMO: -6.74842 LUMO: -0.51974 factor:1 | 1 (-0.22972) | -1 | -1 |
| G: -6257.41721 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.25663 HOMO: -6.13345 LUMO: 0.67756 factor:1 | 1 (-0.47372) | -1 | -1 |
| G: -6257.41721 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.33117 HOMO: -6.48719 LUMO: 0.52790 factor:1 | -1 (0.45174) | -1 | -1 |
| G: -6257.41721 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.39381 HOMO: -6.35930 LUMO: 0.74015 factor:1 | -1 (0.38910) | -1 | -1 |
| G: -6257.41721 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.25571 HOMO: -6.41644 LUMO: 0.22313 factor:1 | -1 (0.52719) | -1 | -1 |
| G: -6257.41721 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.52382 HOMO: -6.85727 LUMO: -0.00272 factor:1 | 1 (-0.74091) | -1 | -1 |
| G: -6257.41721 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.25768 HOMO: -6.84638 LUMO: 0.24762 factor:1 | 1 (-1.47478) | -1 | -1 |
| G: -6257.41721 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12524.11313 HOMO: -6.66951 LUMO: 0.39184 factor:1 | 1 (-2.33022) | -1 | -1 |
| G: -6257.41721 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.87350 HOMO: -6.62597 LUMO: -0.65035 factor:1 | 1 (-2.09060) | -1 | -1 |
| G: -6257.41721 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12524.45047 HOMO: -7.13755 LUMO: 0.45715 factor:1 | 1 (-2.66756) | -1 | -1 |
| G: -6257.41721 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12524.17819 HOMO: -7.12666 LUMO: 0.45171 factor:1 | 1 (-2.39528) | -1 | -1 |
| G: -6257.41721 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.99620 HOMO: -6.46270 LUMO: -0.46259 factor:1 | 1 (-2.21329) | -1 | -1 |
| G: -6257.41721 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.30568 HOMO: -6.36202 LUMO: -0.29660 factor:1 | 1 (-1.52278) | -1 | -1 |
| G: -6257.41721 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12524.13141 HOMO: -6.28583 LUMO: 0.40545 factor:1 | 1 (-2.34851) | -1 | -1 |
| G: -6257.41721 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.64781 HOMO: -6.70761 LUMO: 0.41906 factor:1 | 1 (-1.86491) | -1 | -1 |
| G: -6257.41721 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.39929 HOMO: -6.76203 LUMO: -0.60954 factor:1 | 1 (-1.61638) | -1 | -1 |
| G: -6257.41721 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.36211 HOMO: -6.85999 LUMO: -0.75103 factor:1 | -1 (0.42080) | -1 | -1 |
| G: -6257.41721 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.34856 HOMO: -7.19741 LUMO: -1.00954 factor:1 | -1 (0.43435) | -1 | -1 |
| G: -6257.41721 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.33479 HOMO: -6.58243 LUMO: -0.33470 factor:1 | -1 (0.44812) | -1 | -1 |
| G: -6257.41721 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.99083 HOMO: -7.22190 LUMO: 0.49253 factor:1 | 1 (-0.20792) | -1 | -1 |
| G: -6257.41721 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.26240 HOMO: -7.22462 LUMO: 0.51974 factor:1 | 1 (-0.47949) | -1 | -1 |
| G: -6257.41721 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.24847 HOMO: -7.08584 LUMO: -0.68301 factor:1 | 1 (-0.46556) | -1 | -1 |
| G: -6257.41721 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.85934 HOMO: -6.68584 LUMO: -0.29660 factor:1 | 1 (-0.07644) | -1 | -1 |
| G: -6257.41721 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.36980 HOMO: -6.33753 LUMO: -0.48436 factor:1 | 1 (-0.58690) | -1 | -1 |
| G: -6257.41721 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.06710 HOMO: -7.15932 LUMO: 0.55511 factor:1 | 1 (-0.28420) | -1 | -1 |
| G: -6257.41721 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.91749 HOMO: -6.57427 LUMO: 2.01908 factor:1 | 1 (-0.13459) | -1 | -1 |
| G: -6257.41721 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.22931 HOMO: -6.75659 LUMO: 2.22045 factor:1 | 1 (-0.44640) | -1 | -1 |
| G: -6257.41721 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.85964 HOMO: -6.73482 LUMO: 2.20956 factor:1 | 1 (-0.07674) | -1 | -1 |
| G: -6257.41721 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.96638 HOMO: -6.74026 LUMO: 1.76602 factor:1 | 1 (-2.18347) | -1 | -1 |
| G: -6257.41721 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.06084 HOMO: -6.95523 LUMO: 1.94834 factor:1 | 1 (-1.27793) | -1 | -1 |
| G: -6257.41721 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.24315 HOMO: -6.33209 LUMO: 1.87486 factor:1 | 1 (-1.46024) | -1 | -1 |
| G: -6257.41721 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.99555 HOMO: -6.71033 LUMO: 2.12521 factor:1 | 1 (-2.21264) | -1 | -1 |
| G: -6257.41721 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.99911 HOMO: -6.50080 LUMO: 2.04902 factor:1 | 1 (-2.21620) | -1 | -1 |
| G: -6257.41721 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.12503 HOMO: -6.76475 LUMO: 1.94017 factor:1 | 1 (-1.34212) | -1 | -1 |
| G: -6257.41721 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.64798 HOMO: -6.53073 LUMO: 2.08983 factor:1 | 1 (-1.86507) | -1 | -1 |
| G: -6257.41721 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.72741 HOMO: -6.69944 LUMO: 2.20684 factor:1 | 1 (-0.94451) | -1 | -1 |
| G: -6257.41721 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.18712 HOMO: -6.34570 LUMO: 1.80684 factor:1 | 1 (-1.40422) | -1 | -1 |
| G: -6257.41721 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.38773 HOMO: -6.78380 LUMO: 1.95922 factor:1 | 1 (-1.60482) | -1 | -1 |
| G: -6257.41721 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.44825 HOMO: -6.93618 LUMO: 1.76058 factor:1 | 1 (-0.66535) | -1 | -1 |
| G: -6257.41721 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.33481 HOMO: -6.93346 LUMO: 1.79595 factor:1 | 1 (-0.55190) | -1 | -1 |
| G: -6257.41721 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.30591 HOMO: -6.29671 LUMO: 1.75241 factor:1 | 1 (-0.52300) | -1 | -1 |
| G: -6257.41721 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.01121 HOMO: -6.77019 LUMO: 1.74697 factor:1 | 1 (-0.22830) | -1 | -1 |
| G: -6257.41721 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.52251 HOMO: -6.87360 LUMO: 1.91024 factor:1 | 1 (-0.73961) | -1 | -1 |
| G: -6257.41721 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.10285 HOMO: -6.32665 LUMO: 1.87759 factor:1 | 1 (-1.31994) | -1 | -1 |
| G: -6257.41721 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.32762 HOMO: -6.99877 LUMO: 1.99187 factor:1 | 1 (-0.54472) | -1 | -1 |
| G: -6257.41721 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.10093 HOMO: -6.72665 LUMO: 2.12521 factor:1 | 1 (-0.31802) | -1 | -1 |
| G: -6257.41721 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.33230 HOMO: -6.67767 LUMO: 2.43814 factor:1 | 1 (-0.54940) | -1 | -1 |
| G: -6257.41721 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12519.99125 HOMO: -6.99605 LUMO: 1.79051 factor:1 | -1 (1.79165) | -1 | -1 |
| G: -6257.41721 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12519.98821 HOMO: -6.25046 LUMO: 1.77146 factor:1 | -1 (1.79470) | -1 | -1 |
| G: -6257.41721 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12520.57839 HOMO: -6.30488 LUMO: 1.90480 factor:1 | -1 (1.20451) | -1 | -1 |
| G: -6257.41721 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12520.86689 HOMO: -6.38379 LUMO: 1.68438 factor:1 | -1 (0.91602) | -1 | -1 |
| G: -6257.41721 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.54065 HOMO: -6.78924 LUMO: 2.01364 factor:1 | 1 (-1.75775) | -1 | -1 |
| G: -6257.41721 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.35647 HOMO: -6.15249 LUMO: 1.98643 factor:1 | 1 (-0.57356) | -1 | -1 |
| G: -6257.41721 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.57089 HOMO: -6.19331 LUMO: 2.14154 factor:1 | 1 (-0.78799) | -1 | -1 |
| G: -6257.41721 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.16808 HOMO: -6.05998 LUMO: 2.12521 factor:1 | 1 (-0.38518) | -1 | -1 |
| G: -6257.41721 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.00014 HOMO: -6.67223 LUMO: 1.91840 factor:1 | 1 (-0.21723) | -1 | -1 |
| G: -6257.41721 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.19393 HOMO: -6.79196 LUMO: 2.18507 factor:1 | 1 (-0.41103) | -1 | -1 |
| G: -6257.41721 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12520.87835 HOMO: -6.93346 LUMO: 1.78235 factor:1 | -1 (0.90456) | -1 | -1 |
| G: -6257.41721 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.04390 HOMO: -6.16882 LUMO: 1.80956 factor:1 | -1 (0.73901) | -1 | -1 |
| G: -6257.41721 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.00278 HOMO: -6.72665 LUMO: 2.07895 factor:1 | -1 (0.78012) | -1 | -1 |
| G: -6257.41721 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.29219 HOMO: -6.73210 LUMO: 1.97827 factor:1 | 1 (-1.50928) | -1 | -1 |
| G: -6257.41721 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.53242 HOMO: -6.84638 LUMO: 1.87214 factor:1 | 1 (-0.74951) | -1 | -1 |
| G: -6257.41721 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.03509 HOMO: -6.83006 LUMO: 2.36195 factor:1 | 1 (-1.25219) | -1 | -1 |
| G: -6257.41721 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.22090 HOMO: -6.97700 LUMO: 1.91024 factor:1 | 1 (-0.43799) | -1 | -1 |
| G: -6257.41721 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.56942 HOMO: -6.20420 LUMO: 1.81772 factor:1 | 1 (-0.78652) | -1 | -1 |
| G: -6257.41721 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.32022 HOMO: -7.09129 LUMO: 2.10344 factor:1 | 1 (-0.53732) | 1 | 1 |
| G: -6257.41721 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.33835 HOMO: -6.77564 LUMO: 2.14970 factor:1 | 1 (-0.55544) | -1 | -1 |
| G: -6257.41721 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.32847 HOMO: -6.81645 LUMO: 1.85854 factor:1 | 1 (-0.54556) | -1 | -1 |
| G: -6257.41721 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.46436 HOMO: -6.50896 LUMO: 2.04358 factor:1 | 1 (-0.68145) | -1 | -1 |
| G: -6257.41721 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.13369 HOMO: -6.89264 LUMO: 1.66262 factor:1 | 1 (-0.35078) | -1 | -1 |
| G: -6257.41721 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.11336 HOMO: -6.75931 LUMO: 2.23950 factor:1 | 1 (-0.33046) | -1 | -1 |
| G: -6257.41721 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.26400 HOMO: -6.50080 LUMO: 1.67622 factor:1 | 1 (-0.48110) | -1 | -1 |
| G: -6257.41721 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.01551 HOMO: -6.30216 LUMO: 2.24222 factor:1 | 1 (-0.23260) | -1 | -1 |
| G: -6257.41721 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.14294 HOMO: -7.18108 LUMO: 2.10072 factor:1 | 1 (-0.36003) | 1 | 1 |
| G: -6257.41721 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.33297 HOMO: -6.54162 LUMO: 2.35378 factor:1 | -1 (0.44994) | -1 | -1 |
| G: -6257.41721 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.31362 HOMO: -5.98650 LUMO: 1.48302 factor:1 | -1 (0.46929) | -1 | -1 |
| G: -6257.41721 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.29944 HOMO: -7.15115 LUMO: 2.14970 factor:1 | -1 (0.48346) | 1 | 1 |
| G: -6257.41721 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.28584 HOMO: -6.45454 LUMO: 2.15786 factor:1 | -1 (0.49707) | -1 | -1 |
| G: -6257.41721 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.25239 HOMO: -7.06952 LUMO: 2.14970 factor:1 | -1 (0.53051) | 1 | 1 |
| G: -6257.41721 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.10540 HOMO: -6.93618 LUMO: 1.86942 factor:1 | -1 (0.67751) | -1 | -1 |
| G: -6257.41721 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.61168 HOMO: -6.63141 LUMO: 1.92657 factor:1 | 1 (-0.82878) | -1 | -1 |
| G: -6257.41721 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.60034 HOMO: -6.51441 LUMO: -0.44355 factor:1 | 1 (-0.81743) | -1 | -1 |
| G: -6257.41721 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.24716 HOMO: -6.82734 LUMO: -1.03131 factor:1 | 1 (-0.46425) | -1 | -1 |
| G: -6257.41721 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.29144 HOMO: -6.58788 LUMO: -0.82995 factor:1 | -1 (0.49146) | -1 | -1 |
| G: -6257.41721 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12520.90425 HOMO: -6.43277 LUMO: -0.40817 factor:1 | -1 (0.87866) | -1 | -1 |
| G: -6257.41721 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.09919 HOMO: -6.78924 LUMO: -0.72110 factor:1 | -1 (0.68371) | -1 | -1 |
| G: -6257.41721 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.17898 HOMO: -7.28177 LUMO: 0.36735 factor:1 | -1 (0.60393) | -1 | -1 |
| G: -6257.41721 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.69441 HOMO: -6.47903 LUMO: -0.46259 factor:1 | 1 (-0.91150) | -1 | -1 |
| G: -6257.41721 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.27225 HOMO: -6.67495 LUMO: -0.75376 factor:1 | 1 (-0.48934) | -1 | -1 |
| G: -6257.41721 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.71808 HOMO: -6.71033 LUMO: -0.71838 factor:1 | 1 (-0.93517) | -1 | -1 |
| G: -6257.41721 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.84035 HOMO: -6.79740 LUMO: -0.79185 factor:1 | 1 (-0.05744) | -1 | -1 |
| G: -6257.41721 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.07880 HOMO: -6.08719 LUMO: -0.63675 factor:1 | 1 (-0.29590) | -1 | -1 |
| G: -6257.41721 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.57528 HOMO: -6.84094 LUMO: 0.42994 factor:1 | 1 (-0.79237) | -1 | -1 |
| G: -6257.41721 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.77556 HOMO: -6.59604 LUMO: 0.25851 factor:1 | -1 (0.00735) | -1 | -1 |
| G: -6257.41721 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.15622 HOMO: -6.82462 LUMO: 0.08708 factor:1 | 1 (-0.37331) | -1 | -1 |
| G: -6257.41721 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.96484 HOMO: -6.54706 LUMO: 0.44082 factor:1 | 1 (-0.18194) | -1 | -1 |
| G: -6257.41721 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.80110 HOMO: -6.99333 LUMO: 0.32109 factor:1 | 1 (-1.01820) | -1 | -1 |
| G: -6257.41721 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.57598 HOMO: -6.29944 LUMO: -0.57144 factor:1 | 1 (-0.79308) | -1 | -1 |
| G: -6257.41721 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.26346 HOMO: -6.57699 LUMO: -0.46531 factor:1 | 1 (-0.48055) | -1 | -1 |
| G: -6257.41721 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.07312 HOMO: -6.24773 LUMO: -0.53879 factor:1 | 1 (-0.29021) | -1 | -1 |
| G: -6257.41721 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12520.70291 HOMO: -6.96067 LUMO: -0.67212 factor:1 | -1 (1.07999) | -1 | -1 |
| G: -6257.41721 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.24352 HOMO: -7.24095 LUMO: -0.09252 factor:1 | -1 (0.53938) | -1 | -1 |
| G: -6257.41721 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12520.90101 HOMO: -6.33481 LUMO: -0.46531 factor:1 | -1 (0.88189) | -1 | -1 |
| G: -6257.41721 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.18964 HOMO: -6.43549 LUMO: -0.33198 factor:1 | 1 (-0.40673) | -1 | -1 |
| G: -6257.41721 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.10776 HOMO: -6.53073 LUMO: 0.44899 factor:1 | 1 (-0.32485) | -1 | -1 |
| G: -6257.41721 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.25282 HOMO: -6.69128 LUMO: 0.47620 factor:1 | 1 (-0.46991) | -1 | -1 |
| G: -6257.41721 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.14299 HOMO: -6.65318 LUMO: 0.52246 factor:1 | 1 (-0.36009) | -1 | -1 |
| G: -6257.41721 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.95924 HOMO: -6.71305 LUMO: 0.41089 factor:1 | 1 (-0.17633) | -1 | -1 |
| G: -6257.41721 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.32969 HOMO: -6.70216 LUMO: 0.19864 factor:1 | 1 (-0.54679) | -1 | -1 |
| G: -6257.41721 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.71090 HOMO: -6.41100 LUMO: 0.34558 factor:1 | 1 (-0.92799) | -1 | -1 |
| G: -6257.41721 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.39152 HOMO: -7.01237 LUMO: 0.02993 factor:1 | 1 (-0.60861) | -1 | -1 |
| G: -6257.41721 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.86285 HOMO: -6.85999 LUMO: 0.18776 factor:1 | 1 (-0.07995) | -1 | -1 |
| G: -6257.41721 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.17864 HOMO: -6.62869 LUMO: 0.48708 factor:1 | 1 (-0.39574) | -1 | -1 |
| G: -6257.41721 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.67092 HOMO: -6.43821 LUMO: -0.45715 factor:1 | 1 (-0.88802) | -1 | -1 |
| G: -6257.41721 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.85631 HOMO: -6.43277 LUMO: -0.72110 factor:1 | 1 (-1.07341) | -1 | -1 |
| G: -6257.41721 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.91014 HOMO: -7.10761 LUMO: 0.43266 factor:1 | 1 (-1.12723) | -1 | -1 |
| G: -6257.41721 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.82777 HOMO: -6.57699 LUMO: -0.61498 factor:1 | 1 (-1.04486) | -1 | -1 |
| G: -6257.41721 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.48360 HOMO: -6.82189 LUMO: -0.75648 factor:1 | 1 (-0.70069) | -1 | -1 |
| G: -6257.41721 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.82774 HOMO: -6.55794 LUMO: -0.67212 factor:1 | 1 (-1.04484) | -1 | -1 |
| G: -6257.41721 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.80586 HOMO: -6.69128 LUMO: 1.88575 factor:1 | 1 (-1.02296) | -1 | -1 |
| G: -6257.41721 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.10880 HOMO: -6.65591 LUMO: 1.70888 factor:1 | -1 (0.67411) | -1 | -1 |
| G: -6257.41721 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.21830 HOMO: -6.58788 LUMO: 1.68438 factor:1 | -1 (0.56461) | -1 | -1 |
| G: -6257.41721 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12520.83448 HOMO: -6.46270 LUMO: 1.72520 factor:1 | -1 (0.94843) | -1 | -1 |
| G: -6257.41721 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.38478 HOMO: -6.57427 LUMO: 1.73881 factor:1 | -1 (0.39813) | -1 | -1 |
| G: -6257.41721 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12520.91688 HOMO: -6.45182 LUMO: 1.75241 factor:1 | -1 (0.86603) | -1 | -1 |
| G: -6257.41721 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12520.75040 HOMO: -6.51441 LUMO: 1.78779 factor:1 | -1 (1.03251) | -1 | -1 |
| G: -6257.41721 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12520.96765 HOMO: -6.67495 LUMO: 2.11705 factor:1 | -1 (0.81525) | -1 | -1 |
| G: -6257.41721 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.78579 HOMO: -6.22597 LUMO: 1.96466 factor:1 | 1 (-0.00288) | -1 | -1 |
| G: -6257.41721 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.16363 HOMO: -6.68040 LUMO: 2.30753 factor:1 | -1 (0.61928) | -1 | -1 |
| G: -6257.41721 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.15362 HOMO: -6.65046 LUMO: 2.18235 factor:1 | -1 (0.62929) | -1 | -1 |
| G: -6257.41721 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.39340 HOMO: -6.38651 LUMO: 1.76874 factor:1 | -1 (0.38950) | -1 | -1 |
| G: -6257.41721 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.84914 HOMO: -6.41644 LUMO: 2.09256 factor:1 | 1 (-0.06623) | -1 | -1 |
| G: -6257.41721 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12520.69807 HOMO: -6.14977 LUMO: 2.28031 factor:1 | -1 (1.08484) | -1 | -1 |
| G: -6257.41721 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.79423 HOMO: -6.70489 LUMO: 2.43814 factor:1 | 1 (-0.01132) | -1 | -1 |
| G: -6257.41721 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.77575 HOMO: -6.78924 LUMO: 2.27215 factor:1 | -1 (0.00716) | -1 | -1 |
| G: -6257.41721 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.86163 HOMO: -6.86271 LUMO: 2.31025 factor:1 | 1 (-0.07872) | -1 | -1 |
| G: -6257.41721 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12520.57018 HOMO: -6.51168 LUMO: 2.04630 factor:1 | -1 (1.21273) | -1 | -1 |
| G: -6257.41721 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12520.78409 HOMO: -6.72665 LUMO: 2.13337 factor:1 | -1 (0.99882) | -1 | -1 |
| G: -6257.41721 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12520.64659 HOMO: -6.45998 LUMO: 2.16058 factor:1 | -1 (1.13632) | -1 | -1 |
| G: -6257.41721 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12520.78956 HOMO: -6.83822 LUMO: 2.20684 factor:1 | -1 (0.99335) | -1 | -1 |
| G: -6257.41721 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12520.57924 HOMO: -6.68856 LUMO: 2.19324 factor:1 | -1 (1.20367) | -1 | -1 |
| G: -6257.41721 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.48007 HOMO: -6.71577 LUMO: 2.16058 factor:1 | -1 (0.30284) | -1 | -1 |
| G: -6257.41721 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.71986 HOMO: -6.82462 LUMO: 1.90208 factor:1 | -1 (0.06305) | -1 | -1 |
| G: -6257.41721 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.68832 HOMO: -6.61509 LUMO: 2.23950 factor:1 | -1 (0.09459) | -1 | -1 |
| G: -6257.41721 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.80963 HOMO: -6.73754 LUMO: 1.84221 factor:1 | 1 (-0.02672) | -1 | -1 |
| G: -6257.41721 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.52282 HOMO: -6.56611 LUMO: 1.94561 factor:1 | -1 (0.26009) | -1 | -1 |
| G: -6257.41721 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.24246 HOMO: -6.67767 LUMO: 1.51840 factor:1 | -1 (0.54045) | -1 | -1 |
| G: -6257.41721 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.13242 HOMO: -6.35658 LUMO: 2.16603 factor:1 | -1 (0.65049) | -1 | -1 |
| G: -6257.41721 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.39071 HOMO: -6.35114 LUMO: 2.08983 factor:1 | -1 (0.39220) | -1 | -1 |
| G: -6257.41721 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.47515 HOMO: -6.35114 LUMO: 2.10616 factor:1 | -1 (0.30776) | -1 | -1 |
| G: -6257.41721 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.13343 HOMO: -6.71305 LUMO: 2.01636 factor:1 | -1 (0.64948) | -1 | -1 |
| G: -6257.41721 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.34649 HOMO: -6.24773 LUMO: 1.98915 factor:1 | -1 (0.43642) | -1 | -1 |
| G: -6257.41721 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.91880 HOMO: -6.53617 LUMO: 2.42726 factor:1 | 1 (-0.13589) | -1 | -1 |
| G: -6257.41721 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.17004 HOMO: -6.59332 LUMO: 1.82316 factor:1 | 1 (-0.38714) | -1 | -1 |
| G: -6257.41721 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.70247 HOMO: -6.41372 LUMO: 1.77418 factor:1 | -1 (0.08044) | -1 | -1 |
| G: -6257.41721 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.93322 HOMO: -6.40284 LUMO: 1.88575 factor:1 | 1 (-0.15032) | -1 | -1 |
| G: -6257.41721 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.94160 HOMO: -6.11168 LUMO: 1.70888 factor:1 | 1 (-0.15870) | -1 | -1 |
| G: -6257.41721 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12520.76896 HOMO: -6.44910 LUMO: 2.23405 factor:1 | -1 (1.01395) | -1 | -1 |
| G: -6257.41721 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12520.98725 HOMO: -6.24773 LUMO: 2.12793 factor:1 | -1 (0.79566) | -1 | -1 |
| G: -6257.41721 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.36067 HOMO: -6.07358 LUMO: 1.89663 factor:1 | -1 (0.42224) | -1 | -1 |
| G: -6257.41721 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.43354 HOMO: -6.66679 LUMO: 1.96738 factor:1 | -1 (0.34937) | -1 | -1 |
| G: -6257.41721 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.43852 HOMO: -6.68312 LUMO: 1.78235 factor:1 | -1 (0.34439) | -1 | -1 |
| G: -6257.41721 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.38987 HOMO: -6.70761 LUMO: 1.97555 factor:1 | -1 (0.39304) | -1 | -1 |
| G: -6257.41721 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.57327 HOMO: -6.15794 LUMO: 2.00548 factor:1 | -1 (0.20964) | -1 | -1 |
| G: -6257.41721 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.22633 HOMO: -6.52257 LUMO: 1.96738 factor:1 | -1 (0.55658) | -1 | -1 |
| G: -6257.41721 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.44930 HOMO: -6.25590 LUMO: 1.86670 factor:1 | -1 (0.33361) | -1 | -1 |
| G: -6257.41721 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.13625 HOMO: -6.30216 LUMO: 1.84765 factor:1 | 1 (-0.35334) | -1 | -1 |
| G: -6257.41721 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.87992 HOMO: -6.76747 LUMO: 2.20956 factor:1 | 1 (-0.09701) | -1 | -1 |
| G: -6257.41721 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.27954 HOMO: -6.14161 LUMO: 1.80684 factor:1 | 1 (-0.49664) | -1 | -1 |
| G: -6257.41721 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.04751 HOMO: -6.81373 LUMO: 1.91024 factor:1 | 1 (-0.26460) | -1 | -1 |
| G: -6257.41721 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.37865 HOMO: -6.81917 LUMO: 2.34834 factor:1 | 1 (-0.59574) | -1 | -1 |
| G: -6257.41721 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.40431 HOMO: -6.72121 LUMO: 1.90208 factor:1 | -1 (0.37859) | -1 | -1 |
| G: -6257.41721 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.13532 HOMO: -7.51851 LUMO: 0.26939 factor:1 | 1 (-0.35241) | -1 | -1 |
| G: -6257.41721 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.55790 HOMO: -6.65318 LUMO: -0.57144 factor:1 | -1 (0.22501) | -1 | -1 |
| G: -6257.41721 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.82321 HOMO: -6.77564 LUMO: -0.72654 factor:1 | 1 (-0.04030) | -1 | -1 |
| G: -6257.41721 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.30137 HOMO: -6.80557 LUMO: -0.60954 factor:1 | 1 (-0.51846) | -1 | -1 |
| G: -6257.41721 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.57545 HOMO: -7.35524 LUMO: 0.27483 factor:1 | -1 (0.20746) | -1 | -1 |
| G: -6257.41721 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.80040 HOMO: -6.94979 LUMO: -0.83811 factor:1 | 1 (-0.01750) | -1 | -1 |
| G: -6257.41721 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.60731 HOMO: -6.13345 LUMO: -0.67212 factor:1 | -1 (0.17560) | -1 | -1 |
| G: -6257.41721 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.83167 HOMO: -6.47359 LUMO: -0.59321 factor:1 | 1 (-0.04876) | -1 | -1 |
| G: -6257.41721 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.06465 HOMO: -6.52257 LUMO: -0.54695 factor:1 | 1 (-0.28175) | -1 | -1 |
| G: -6257.41721 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.02860 HOMO: -6.61781 LUMO: -0.69661 factor:1 | 1 (-0.24569) | -1 | -1 |
| G: -6257.41721 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.22449 HOMO: -6.77564 LUMO: -0.80001 factor:1 | 1 (-0.44159) | -1 | -1 |
| G: -6257.41721 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.27791 HOMO: -7.35252 LUMO: -1.00410 factor:1 | 1 (-0.49500) | -1 | -1 |
| G: -6257.41721 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.64649 HOMO: -6.35386 LUMO: -0.38912 factor:1 | 1 (-0.86358) | -1 | -1 |
| G: -6257.41721 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.78986 HOMO: -6.80285 LUMO: -0.52246 factor:1 | 1 (-1.00696) | -1 | -1 |
| G: -6257.41721 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.75827 HOMO: -7.23279 LUMO: 0.30477 factor:1 | 1 (-0.97536) | -1 | -1 |
| G: -6257.41721 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.50164 HOMO: -7.13483 LUMO: -0.76192 factor:1 | 1 (-0.71873) | -1 | -1 |
| G: -6257.41721 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.42621 HOMO: -6.71849 LUMO: -0.48164 factor:1 | 1 (-0.64330) | -1 | -1 |
| G: -6257.41721 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.12842 HOMO: -6.85455 LUMO: -0.69389 factor:1 | -1 (0.65449) | -1 | -1 |
| G: -6257.41721 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.13451 HOMO: -6.96339 LUMO: -0.73743 factor:1 | -1 (0.64839) | -1 | -1 |
| G: -6257.41721 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.12891 HOMO: -7.50490 LUMO: 0.28844 factor:1 | -1 (0.65400) | -1 | -1 |
| G: -6257.41721 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.09672 HOMO: -6.63958 LUMO: -0.50069 factor:1 | -1 (0.68619) | -1 | -1 |
| G: -6257.41721 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.09557 HOMO: -6.78924 LUMO: -0.69661 factor:1 | -1 (0.68733) | -1 | -1 |
| G: -6257.41721 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12520.82395 HOMO: -7.44776 LUMO: 0.33742 factor:1 | -1 (0.95896) | -1 | -1 |
| G: -6257.41721 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.29133 HOMO: -6.15249 LUMO: 0.66396 factor:1 | -1 (0.49157) | -1 | -1 |
| G: -6257.41721 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.41155 HOMO: -6.17426 LUMO: 0.55511 factor:1 | -1 (0.37135) | -1 | -1 |
| G: -6257.41721 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.48810 HOMO: -6.83550 LUMO: 0.28844 factor:1 | -1 (0.29481) | -1 | -1 |
| G: -6257.41721 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.38206 HOMO: -6.32393 LUMO: 0.47620 factor:1 | -1 (0.40085) | -1 | -1 |
| G: -6257.41721 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12520.95013 HOMO: -6.32937 LUMO: 0.45987 factor:1 | -1 (0.83278) | -1 | -1 |
| G: -6257.41721 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.37615 HOMO: -7.37429 LUMO: 0.09252 factor:1 | -1 (0.40676) | -1 | -1 |
| G: -6257.41721 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.30322 HOMO: -6.54434 LUMO: -0.39729 factor:1 | -1 (0.47968) | -1 | -1 |
| G: -6257.41721 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.08004 HOMO: -7.35524 LUMO: 0.28028 factor:1 | -1 (0.70287) | -1 | -1 |
| G: -6257.41721 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12520.99448 HOMO: -6.95523 LUMO: -0.86804 factor:1 | -1 (0.78842) | -1 | -1 |
| G: -6257.41721 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12520.64174 HOMO: -6.63958 LUMO: -0.65307 factor:1 | -1 (1.14116) | -1 | -1 |
| G: -6257.41721 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.38494 HOMO: -6.73482 LUMO: -0.67212 factor:1 | -1 (0.39797) | -1 | -1 |
| G: -6257.41721 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.07364 HOMO: -6.37835 LUMO: -0.53606 factor:1 | -1 (0.70926) | -1 | -1 |
| G: -6257.41721 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.24091 HOMO: -6.71849 LUMO: -0.61226 factor:1 | -1 (0.54200) | -1 | -1 |
| G: -6257.41721 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.43403 HOMO: -6.68584 LUMO: -1.11022 factor:1 | -1 (0.34888) | -1 | -1 |
| G: -6257.41721 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.66144 HOMO: -6.80285 LUMO: -0.79185 factor:1 | -1 (0.12147) | -1 | -1 |
| G: -6257.41721 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.16610 HOMO: -7.14571 LUMO: -0.94696 factor:1 | 1 (-0.38319) | -1 | -1 |
| G: -6257.41721 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.10242 HOMO: -7.16204 LUMO: -0.66124 factor:1 | 1 (-0.31952) | -1 | -1 |
| G: -6257.41721 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.11293 HOMO: -6.54978 LUMO: -0.54967 factor:1 | 1 (-0.33002) | -1 | -1 |
| G: -6257.41721 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.76734 HOMO: -6.75114 LUMO: -0.70750 factor:1 | -1 (0.01556) | -1 | -1 |
| G: -6257.41721 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.90438 HOMO: -7.22190 LUMO: 0.39184 factor:1 | 1 (-0.12147) | -1 | -1 |
| G: -6257.41721 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.83140 HOMO: -7.43959 LUMO: 0.30477 factor:1 | 1 (-0.04849) | -1 | -1 |
| G: -6257.41721 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.77567 HOMO: -6.87360 LUMO: -0.77552 factor:1 | -1 (0.00724) | -1 | -1 |
| G: -6257.41721 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.54625 HOMO: -6.82734 LUMO: -0.59593 factor:1 | -1 (0.23666) | -1 | -1 |
| G: -6257.41721 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.64500 HOMO: -6.65318 LUMO: -0.46259 factor:1 | -1 (0.13791) | -1 | -1 |
| G: -6257.41721 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.81880 HOMO: -7.05863 LUMO: -1.17009 factor:1 | 1 (-0.03589) | -1 | -1 |
| G: -6257.41721 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.93611 HOMO: -6.57427 LUMO: -0.48708 factor:1 | 1 (-0.15320) | -1 | -1 |
| G: -6257.41721 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.87099 HOMO: -6.60420 LUMO: -0.38096 factor:1 | 1 (-0.08808) | -1 | -1 |
| G: -6257.41721 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.28226 HOMO: -6.72121 LUMO: -0.66668 factor:1 | 1 (-0.49936) | -1 | -1 |
| G: -6257.41721 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.59685 HOMO: -6.52257 LUMO: -0.19320 factor:1 | 1 (-0.81395) | -1 | -1 |
| G: -6257.41721 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.49753 HOMO: -6.28039 LUMO: -0.27211 factor:1 | 1 (-0.71463) | -1 | -1 |
| G: -6257.41721 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.28264 HOMO: -6.71849 LUMO: -0.42722 factor:1 | 1 (-0.49974) | -1 | -1 |
| G: -6257.41721 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.59933 HOMO: -6.27495 LUMO: 0.27756 factor:1 | 1 (-0.81642) | -1 | -1 |
| G: -6257.41721 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.39603 HOMO: -6.21780 LUMO: 0.46531 factor:1 | 1 (-0.61313) | -1 | -1 |
| G: -6257.41721 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.08694 HOMO: -6.52257 LUMO: -0.64491 factor:1 | 1 (-0.30403) | -1 | -1 |
| G: -6257.41721 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.57189 HOMO: -6.73754 LUMO: 1.83133 factor:1 | 1 (-1.78899) | -1 | -1 |
| G: -6257.41721 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.69528 HOMO: -6.67223 LUMO: 1.88847 factor:1 | 1 (-0.91237) | -1 | -1 |
| G: -6257.41721 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.44295 HOMO: -6.82189 LUMO: 1.59187 factor:1 | 1 (-0.66004) | -1 | -1 |
| G: -6257.41721 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.30410 HOMO: -6.43277 LUMO: 1.76330 factor:1 | 1 (-1.52120) | -1 | -1 |
| G: -6257.41721 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.60521 HOMO: -6.48175 LUMO: 1.77962 factor:1 | 1 (-0.82230) | -1 | -1 |
| G: -6257.41721 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.58257 HOMO: -6.50352 LUMO: 1.68438 factor:1 | 1 (-0.79966) | -1 | -1 |
| G: -6257.41721 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.38539 HOMO: -6.31576 LUMO: 2.03813 factor:1 | 1 (-0.60249) | -1 | -1 |
| G: -6257.41721 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.56417 HOMO: -6.27495 LUMO: 1.99459 factor:1 | 1 (-0.78127) | -1 | -1 |
| G: -6257.41721 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.58934 HOMO: -6.23957 LUMO: 2.17147 factor:1 | 1 (-0.80644) | -1 | -1 |
| G: -6257.41721 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.69413 HOMO: -6.78108 LUMO: 2.16875 factor:1 | 1 (-0.91123) | -1 | -1 |
| G: -6257.41721 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.28523 HOMO: -6.34297 LUMO: 2.10344 factor:1 | 1 (-0.50232) | -1 | -1 |
| G: -6257.41721 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.39241 HOMO: -6.30216 LUMO: 2.00004 factor:1 | 1 (-0.60951) | -1 | -1 |
| G: -6257.41721 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.30256 HOMO: -6.72665 LUMO: 2.09528 factor:1 | 1 (-0.51966) | -1 | -1 |
| G: -6257.41721 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.46583 HOMO: -6.86543 LUMO: 1.91568 factor:1 | 1 (-0.68292) | -1 | -1 |
| G: -6257.41721 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.41018 HOMO: -5.83956 LUMO: 1.89391 factor:1 | 1 (-0.62728) | -1 | -1 |
| G: -6257.41721 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.17611 HOMO: -6.42189 LUMO: 2.03269 factor:1 | 1 (-0.39320) | -1 | -1 |
| G: -6257.41721 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.14789 HOMO: -6.07630 LUMO: 1.80956 factor:1 | 1 (-0.36499) | -1 | -1 |
| G: -6257.41721 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12520.81581 HOMO: -6.43277 LUMO: 1.81772 factor:1 | -1 (0.96709) | -1 | -1 |
| G: -6257.41721 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12520.72553 HOMO: -7.03959 LUMO: 1.78779 factor:1 | -1 (1.05738) | -1 | -1 |
| G: -6257.41721 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.12842 HOMO: -6.72121 LUMO: 2.29664 factor:1 | -1 (0.65449) | -1 | -1 |
| G: -6257.41721 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.01106 HOMO: -6.62869 LUMO: 2.04630 factor:1 | -1 (0.77185) | -1 | -1 |
| G: -6257.41721 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.64194 HOMO: -6.63958 LUMO: 1.84221 factor:1 | 1 (-0.85904) | -1 | -1 |
| G: -6257.41721 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.31394 HOMO: -6.70761 LUMO: 1.67350 factor:1 | 1 (-0.53103) | -1 | -1 |
| G: -6257.41721 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12520.72142 HOMO: -6.00283 LUMO: 1.64357 factor:1 | -1 (1.06149) | -1 | -1 |
| G: -6257.41721 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.03982 HOMO: -6.48719 LUMO: 1.70343 factor:1 | -1 (0.74309) | -1 | -1 |
| G: -6257.41721 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.59707 HOMO: -6.13345 LUMO: 1.44492 factor:1 | 1 (-0.81416) | -1 | -1 |
| G: -6257.41721 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.60611 HOMO: -6.11168 LUMO: 1.70071 factor:1 | 1 (-0.82320) | -1 | -1 |
| G: -6257.41721 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.31415 HOMO: -6.09535 LUMO: 1.82316 factor:1 | 1 (-0.53125) | -1 | -1 |
| G: -6257.41721 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.80106 HOMO: -6.81101 LUMO: 1.63540 factor:1 | 1 (-0.01815) | -1 | -1 |
| G: -6257.41721 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.04800 HOMO: -6.80013 LUMO: 2.12249 factor:1 | 1 (-0.26509) | -1 | -1 |
| G: -6257.41721 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.38154 HOMO: -6.48447 LUMO: 1.94561 factor:1 | -1 (0.40137) | -1 | -1 |
| G: -6257.41721 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.22290 HOMO: -6.72393 LUMO: 2.06534 factor:1 | -1 (0.56001) | -1 | -1 |
| G: -6257.41721 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.26619 HOMO: -6.34570 LUMO: 1.98915 factor:1 | -1 (0.51672) | -1 | -1 |
| G: -6257.41721 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.31169 HOMO: -6.31304 LUMO: 1.87759 factor:1 | -1 (0.47122) | -1 | -1 |
| G: -6257.41721 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12520.97179 HOMO: -6.77564 LUMO: 1.81228 factor:1 | -1 (0.81112) | -1 | -1 |
| G: -6257.41721 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.08839 HOMO: -6.58516 LUMO: 2.34834 factor:1 | -1 (0.69452) | -1 | -1 |
| G: -6257.41721 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.23130 HOMO: -6.68040 LUMO: 2.20412 factor:1 | -1 (0.55160) | -1 | -1 |
| G: -6257.41721 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.26377 HOMO: -6.20964 LUMO: 2.17147 factor:1 | -1 (0.51914) | -1 | -1 |
| G: -6257.41721 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.30820 HOMO: -6.54706 LUMO: 2.03813 factor:1 | 1 (-0.52529) | -1 | -1 |
| G: -6257.41721 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.40931 HOMO: -6.54162 LUMO: 2.17419 factor:1 | 1 (-0.62641) | -1 | -1 |
| G: -6257.41721 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.19854 HOMO: -6.75659 LUMO: 2.22589 factor:1 | -1 (0.58436) | -1 | -1 |
| G: -6257.41721 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.35161 HOMO: -6.59604 LUMO: 2.59325 factor:1 | -1 (0.43130) | -1 | -1 |
| G: -6257.41721 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.06871 HOMO: -6.11712 LUMO: 2.02181 factor:1 | 1 (-0.28580) | -1 | -1 |
| G: -6257.41721 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.04452 HOMO: -6.63141 LUMO: 2.09256 factor:1 | 1 (-0.26161) | -1 | -1 |
| G: -6257.41721 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.07567 HOMO: -6.61781 LUMO: 1.86126 factor:1 | 1 (-0.29277) | -1 | -1 |
| G: -6257.41721 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.23423 HOMO: -6.63958 LUMO: 1.77146 factor:1 | 1 (-0.45133) | -1 | -1 |
| G: -6257.41721 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.89606 HOMO: -6.60420 LUMO: 1.54561 factor:1 | 1 (-2.11315) | -1 | -1 |
| G: -6257.41721 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.11518 HOMO: -6.52529 LUMO: 2.05174 factor:1 | 1 (-1.33227) | -1 | -1 |
| G: -6257.41721 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.88746 HOMO: -6.80285 LUMO: 2.13609 factor:1 | 1 (-2.10456) | -1 | -1 |
| G: -6257.41721 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.58035 HOMO: -6.51168 LUMO: 2.25855 factor:1 | 1 (-1.79745) | -1 | -1 |
| G: -6257.41721 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.77128 HOMO: -6.64774 LUMO: 2.46263 factor:1 | 1 (-0.98837) | -1 | -1 |
| G: -6257.41721 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.02312 HOMO: -6.40828 LUMO: 1.99732 factor:1 | 1 (-1.24021) | -1 | -1 |
| G: -6257.41721 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.35826 HOMO: -5.97562 LUMO: 1.56465 factor:1 | 1 (-1.57535) | -1 | -1 |
| G: -6257.41721 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.30741 HOMO: -6.75659 LUMO: 2.23405 factor:1 | 1 (-0.52450) | -1 | -1 |
| G: -6257.41721 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.08291 HOMO: -6.68584 LUMO: 2.09528 factor:1 | 1 (-0.30001) | -1 | -1 |
| G: -6257.41721 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.85461 HOMO: -6.86543 LUMO: 1.95106 factor:1 | 1 (-0.07170) | -1 | -1 |
| G: -6257.41721 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.55727 HOMO: -6.47359 LUMO: 1.82316 factor:1 | -1 (0.22564) | -1 | -1 |
| G: -6257.41721 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.02626 HOMO: -6.87632 LUMO: 2.08439 factor:1 | 1 (-0.24335) | -1 | -1 |
| G: -6257.41721 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12520.85138 HOMO: -6.33753 LUMO: 2.16603 factor:1 | -1 (0.93153) | -1 | -1 |
| G: -6257.41721 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12520.88790 HOMO: -6.92258 LUMO: 1.72248 factor:1 | -1 (0.89501) | -1 | -1 |
| G: -6257.41721 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.19171 HOMO: -6.62597 LUMO: 2.10344 factor:1 | -1 (0.59119) | -1 | -1 |
| G: -6257.41721 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.07617 HOMO: -6.63141 LUMO: 1.94017 factor:1 | -1 (0.70673) | -1 | -1 |
| G: -6257.41721 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12520.86537 HOMO: -6.48447 LUMO: 1.91840 factor:1 | -1 (0.91754) | -1 | -1 |
| G: -6257.41721 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.21824 HOMO: -6.41372 LUMO: 1.61364 factor:1 | -1 (0.56466) | -1 | -1 |
| G: -6257.41721 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12520.58871 HOMO: -6.37291 LUMO: 1.79051 factor:1 | -1 (1.19420) | -1 | -1 |
| G: -6257.41721 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12520.44783 HOMO: -6.13073 LUMO: 1.77962 factor:1 | -1 (1.33507) | -1 | -1 |
| G: -6257.41721 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.18450 HOMO: -6.13073 LUMO: 1.98915 factor:1 | -1 (0.59841) | -1 | -1 |
| G: -6257.41721 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.34480 HOMO: -6.44094 LUMO: 1.58370 factor:1 | -1 (0.43810) | -1 | -1 |
| G: -6257.41721 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.15830 HOMO: -6.87087 LUMO: -0.82995 factor:1 | -1 (0.62461) | -1 | -1 |
| G: -6257.41721 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.22714 HOMO: -6.67223 LUMO: 1.08029 factor:1 | -1 (0.55577) | -1 | -1 |
| G: -6257.41721 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.06975 HOMO: -6.82462 LUMO: 0.91702 factor:1 | -1 (0.71316) | -1 | -1 |
| G: -6257.41721 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.14504 HOMO: -6.65863 LUMO: 1.52656 factor:1 | -1 (0.63786) | -1 | -1 |
| G: -6257.41721 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.00194 HOMO: -6.78924 LUMO: 0.86260 factor:1 | -1 (0.78097) | -1 | -1 |
| G: -6257.41721 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.16994 HOMO: -6.68584 LUMO: 0.94424 factor:1 | -1 (0.61296) | -1 | -1 |
| G: -6257.41721 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12520.84000 HOMO: -6.58788 LUMO: 1.00138 factor:1 | -1 (0.94290) | -1 | -1 |
| G: -6257.41721 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.22940 HOMO: -6.79740 LUMO: 0.91430 factor:1 | -1 (0.55351) | -1 | -1 |
| G: -6257.41721 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.87594 HOMO: -6.67223 LUMO: 0.80274 factor:1 | 1 (-0.09304) | -1 | -1 |
| G: -6257.41721 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.52913 HOMO: -6.95251 LUMO: 0.90614 factor:1 | -1 (0.25377) | -1 | -1 |
| G: -6257.41721 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.46840 HOMO: -7.19469 LUMO: 1.34152 factor:1 | -1 (0.31451) | -1 | -1 |
| G: -6257.41721 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.70008 HOMO: -6.59332 LUMO: -0.76464 factor:1 | -1 (0.08283) | -1 | -1 |
| G: -6257.41721 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12520.67206 HOMO: -6.77564 LUMO: -0.90886 factor:1 | -1 (1.11085) | -1 | -1 |
| G: -6257.41721 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12520.81837 HOMO: -6.57971 LUMO: -0.41633 factor:1 | -1 (0.96453) | -1 | -1 |
| G: -6257.41721 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12520.58835 HOMO: -6.68856 LUMO: -0.58232 factor:1 | -1 (1.19455) | -1 | -1 |
| G: -6257.41721 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12520.71219 HOMO: -6.87087 LUMO: -0.71022 factor:1 | -1 (1.07071) | -1 | -1 |
| G: -6257.41721 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12520.34840 HOMO: -6.67767 LUMO: -0.74559 factor:1 | -1 (1.43450) | -1 | -1 |
| G: -6257.41721 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12520.79644 HOMO: -6.68040 LUMO: -0.65307 factor:1 | -1 (0.98647) | -1 | -1 |
| G: -6257.41721 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.41063 HOMO: -6.32937 LUMO: 0.80274 factor:1 | -1 (0.37228) | -1 | -1 |
| G: -6257.41721 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.45985 HOMO: -6.29671 LUMO: 0.82723 factor:1 | -1 (0.32305) | -1 | -1 |
| G: -6257.41721 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12520.22299 HOMO: -6.67767 LUMO: 0.59321 factor:1 | -1 (1.55992) | -1 | -1 |
| G: -6257.41721 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12520.26223 HOMO: -6.77836 LUMO: 0.50341 factor:1 | -1 (1.52068) | -1 | -1 |
| G: -6257.41721 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.55009 HOMO: -6.61781 LUMO: 0.42450 factor:1 | -1 (0.23282) | -1 | -1 |
| G: -6257.41721 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.48652 HOMO: -6.83278 LUMO: 0.39457 factor:1 | -1 (0.29639) | -1 | -1 |
| G: -6257.41721 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12520.23831 HOMO: -6.56883 LUMO: 0.64219 factor:1 | -1 (1.54460) | -1 | -1 |
| G: -6257.41721 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12520.17224 HOMO: -6.71577 LUMO: 0.40001 factor:1 | -1 (1.61067) | -1 | -1 |
| G: -6257.41721 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12519.76121 HOMO: -6.86543 LUMO: -0.74287 factor:1 | -1 (2.02170) | -1 | -1 |
| G: -6257.41721 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12519.74943 HOMO: -6.68584 LUMO: -0.69389 factor:1 | -1 (2.03348) | -1 | -1 |
| G: -6257.41721 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12519.98584 HOMO: -6.61237 LUMO: -0.48980 factor:1 | -1 (1.79707) | -1 | -1 |
| G: -6257.41721 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.36091 HOMO: -6.80285 LUMO: -0.58232 factor:1 | -1 (0.42199) | -1 | -1 |
| G: -6257.41721 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.46875 HOMO: -6.88992 LUMO: -0.70205 factor:1 | -1 (0.31416) | -1 | -1 |
| G: -6257.41721 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.57346 HOMO: -6.95251 LUMO: -0.71838 factor:1 | -1 (0.20945) | -1 | -1 |
| G: -6257.41721 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.58103 HOMO: -7.52123 LUMO: 0.27211 factor:1 | -1 (0.20188) | -1 | -1 |
| G: -6257.41721 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.39675 HOMO: -6.76747 LUMO: -0.74015 factor:1 | -1 (0.38616) | -1 | -1 |
| G: -6257.41721 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.22173 HOMO: -6.55250 LUMO: -0.49797 factor:1 | -1 (0.56118) | -1 | -1 |
| G: -6257.41721 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.26886 HOMO: -6.50896 LUMO: -0.46804 factor:1 | -1 (0.51405) | -1 | -1 |
| G: -6257.41721 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.32771 HOMO: -7.45320 LUMO: 0.08436 factor:1 | -1 (0.45519) | -1 | -1 |
| G: -6257.41721 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.19694 HOMO: -6.82462 LUMO: -0.70477 factor:1 | -1 (0.58597) | -1 | -1 |
| G: -6257.41721 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.04793 HOMO: -6.57155 LUMO: -0.43538 factor:1 | -1 (0.73498) | -1 | -1 |
| G: -6257.41721 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12520.87606 HOMO: -6.72665 LUMO: -0.55239 factor:1 | -1 (0.90685) | -1 | -1 |
| G: -6257.41721 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12520.52231 HOMO: -7.05319 LUMO: -1.08573 factor:1 | -1 (1.26059) | -1 | -1 |
| G: -6257.41721 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12520.96232 HOMO: -6.56067 LUMO: -0.45715 factor:1 | -1 (0.82059) | -1 | -1 |
| G: -6257.41721 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.92920 HOMO: -6.76475 LUMO: -0.53879 factor:1 | 1 (-0.14629) | -1 | -1 |
| G: -6257.41721 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.24115 HOMO: -6.67223 LUMO: -0.45987 factor:1 | 1 (-0.45824) | -1 | -1 |
| G: -6257.41721 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.44921 HOMO: -6.44094 LUMO: -0.72110 factor:1 | -1 (0.33369) | -1 | -1 |
| G: -6257.41721 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.72715 HOMO: -6.66951 LUMO: -0.67756 factor:1 | -1 (0.05576) | -1 | -1 |
| G: -6257.41721 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12520.59663 HOMO: -6.69400 LUMO: -0.62858 factor:1 | -1 (1.18628) | -1 | -1 |
| G: -6257.41721 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12520.65255 HOMO: -6.51985 LUMO: -0.37007 factor:1 | -1 (1.13036) | -1 | -1 |
| G: -6257.41721 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12520.55924 HOMO: -5.98378 LUMO: 0.78641 factor:1 | -1 (1.22367) | -1 | -1 |
| G: -6257.41721 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12520.36843 HOMO: -6.11440 LUMO: 0.71294 factor:1 | -1 (1.41448) | -1 | -1 |
| G: -6257.41721 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12520.93723 HOMO: -6.45182 LUMO: 0.63947 factor:1 | -1 (0.84568) | -1 | -1 |
| G: -6257.41721 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12520.82890 HOMO: -6.78924 LUMO: 0.37007 factor:1 | -1 (0.95400) | -1 | -1 |
| G: -6257.41721 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.28263 HOMO: -6.63686 LUMO: 0.54423 factor:1 | -1 (0.50028) | -1 | -1 |
| G: -6257.41721 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.37245 HOMO: -6.66679 LUMO: 0.48708 factor:1 | -1 (0.41046) | -1 | -1 |
| G: -6257.41721 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.98441 HOMO: -6.81917 LUMO: 0.31021 factor:1 | 1 (-0.20150) | -1 | -1 |
| G: -6257.41721 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.24923 HOMO: -6.28583 LUMO: 0.44899 factor:1 | 1 (-0.46632) | -1 | -1 |
| G: -6257.41721 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.19440 HOMO: -6.61237 LUMO: 0.49525 factor:1 | 1 (-0.41149) | -1 | -1 |
| G: -6257.41721 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.41198 HOMO: -7.08857 LUMO: 0.38368 factor:1 | 1 (-0.62907) | -1 | -1 |
| G: -6257.41721 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.81047 HOMO: -6.53890 LUMO: -0.68845 factor:1 | 1 (-0.02757) | -1 | -1 |
| G: -6257.41721 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.58247 HOMO: -6.56611 LUMO: -0.66396 factor:1 | -1 (0.20044) | -1 | -1 |
| G: -6257.41721 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.53185 HOMO: -6.04909 LUMO: -0.59865 factor:1 | -1 (0.25105) | -1 | -1 |
| G: -6257.41721 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.46959 HOMO: -6.74842 LUMO: -0.77825 factor:1 | -1 (0.31331) | -1 | -1 |
| G: -6257.41721 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.82887 HOMO: -6.82462 LUMO: -0.61498 factor:1 | 1 (-0.04596) | -1 | -1 |
| G: -6257.41721 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.74184 HOMO: -7.40694 LUMO: 0.32926 factor:1 | -1 (0.04106) | -1 | -1 |
| G: -6257.41721 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.45104 HOMO: -6.80557 LUMO: -0.57416 factor:1 | -1 (0.33187) | -1 | -1 |
| G: -6257.41721 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.10738 HOMO: -6.76747 LUMO: -0.67484 factor:1 | -1 (0.67552) | -1 | -1 |
| G: -6257.41721 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.78345 HOMO: -7.23279 LUMO: 0.48980 factor:1 | 1 (-0.00054) | -1 | -1 |
| G: -6257.41721 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.42434 HOMO: -6.62869 LUMO: -0.24762 factor:1 | -1 (0.35856) | -1 | -1 |
| G: -6257.41721 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.27369 HOMO: -6.65863 LUMO: -0.28028 factor:1 | 1 (-0.49078) | -1 | -1 |
| G: -6257.41721 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.45916 HOMO: -6.50352 LUMO: -0.44899 factor:1 | 1 (-0.67626) | -1 | -1 |
| G: -6257.41721 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.45233 HOMO: -6.62053 LUMO: -0.88437 factor:1 | 1 (-1.66942) | -1 | -1 |
| G: -6257.41721 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.61068 HOMO: -6.73754 LUMO: -0.77825 factor:1 | 1 (-0.82777) | -1 | -1 |
| G: -6257.41721 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.54016 HOMO: -7.24639 LUMO: 0.35647 factor:1 | 1 (-1.75726) | -1 | -1 |
| G: -6257.41721 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.47974 HOMO: -6.46270 LUMO: -0.48164 factor:1 | 1 (-0.69683) | -1 | -1 |
| G: -6257.41721 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.37858 HOMO: -6.14161 LUMO: -0.66396 factor:1 | 1 (-1.59568) | -1 | -1 |
| G: -6257.41721 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.39815 HOMO: -6.63414 LUMO: 1.51295 factor:1 | 1 (-1.61524) | -1 | -1 |
| G: -6257.41721 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.12405 HOMO: -6.52529 LUMO: 1.65989 factor:1 | 1 (-1.34114) | -1 | -1 |
| G: -6257.41721 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.19010 HOMO: -6.63686 LUMO: 1.64629 factor:1 | 1 (-0.40719) | -1 | -1 |
| G: -6257.41721 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.30822 HOMO: -6.49808 LUMO: 1.60003 factor:1 | 1 (-0.52532) | -1 | -1 |
| G: -6257.41721 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.88647 HOMO: -6.85183 LUMO: 1.96194 factor:1 | 1 (-0.10357) | -1 | -1 |
| G: -6257.41721 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.44401 HOMO: -6.90081 LUMO: 1.82316 factor:1 | 1 (-0.66110) | -1 | -1 |
| G: -6257.41721 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.93195 HOMO: -6.20147 LUMO: 1.95106 factor:1 | 1 (-2.14905) | -1 | -1 |
| G: -6257.41721 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.89900 HOMO: -7.05047 LUMO: 1.94289 factor:1 | 1 (-2.11609) | -1 | -1 |
| G: -6257.41721 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.98254 HOMO: -6.11440 LUMO: 1.83949 factor:1 | 1 (-2.19963) | -1 | -1 |
| G: -6257.41721 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12524.44698 HOMO: -6.65046 LUMO: 1.59187 factor:1 | 1 (-2.66408) | -1 | -1 |
| G: -6257.41721 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.15485 HOMO: -6.81917 LUMO: 2.41365 factor:1 | 1 (-1.37194) | -1 | -1 |
| G: -6257.41721 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.74330 HOMO: -6.40284 LUMO: 2.48984 factor:1 | 1 (-1.96039) | -1 | -1 |
| G: -6257.41721 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12524.03043 HOMO: -7.04775 LUMO: 2.31025 factor:1 | 1 (-2.24752) | -1 | -1 |
| G: -6257.41721 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.25072 HOMO: -6.64774 LUMO: 2.20140 factor:1 | 1 (-1.46781) | -1 | -1 |
| G: -6257.41721 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.72581 HOMO: -6.72393 LUMO: 2.28304 factor:1 | 1 (-0.94290) | -1 | -1 |
| G: -6257.41721 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.67762 HOMO: -6.35114 LUMO: 1.84765 factor:1 | 1 (-0.89471) | -1 | -1 |
| G: -6257.41721 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.39013 HOMO: -6.41100 LUMO: 1.74697 factor:1 | 1 (-0.60722) | -1 | -1 |
| G: -6257.41721 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.40376 HOMO: -6.34297 LUMO: 1.55921 factor:1 | 1 (-0.62085) | -1 | -1 |
| G: -6257.41721 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.29108 HOMO: -6.31848 LUMO: 1.67622 factor:1 | 1 (-0.50817) | -1 | -1 |
| G: -6257.41721 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.43516 HOMO: -6.50896 LUMO: 2.02725 factor:1 | 1 (-0.65226) | -1 | -1 |
| G: -6257.41721 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12524.04883 HOMO: -6.28583 LUMO: 2.00548 factor:1 | 1 (-2.26592) | -1 | -1 |
| G: -6257.41721 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.25368 HOMO: -6.67495 LUMO: 1.92384 factor:1 | 1 (-1.47078) | -1 | -1 |
| G: -6257.41721 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12524.07400 HOMO: -6.17154 LUMO: 2.39732 factor:1 | 1 (-2.29109) | -1 | -1 |
| G: -6257.41721 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12524.18385 HOMO: -6.84911 LUMO: 2.24766 factor:1 | 1 (-2.40094) | -1 | -1 |
| G: -6257.41721 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.33308 HOMO: -6.77564 LUMO: 2.38372 factor:1 | 1 (-1.55018) | -1 | -1 |
| G: -6257.41721 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12524.02298 HOMO: -6.18243 LUMO: 2.40821 factor:1 | 1 (-2.24007) | -1 | -1 |
| G: -6257.41721 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.07460 HOMO: -6.40828 LUMO: 2.22589 factor:1 | 1 (-1.29170) | -1 | -1 |
| G: -6257.41721 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.27254 HOMO: -6.74570 LUMO: 1.88303 factor:1 | 1 (-1.48963) | -1 | -1 |
| G: -6257.41721 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.37452 HOMO: -6.29944 LUMO: 2.05174 factor:1 | -1 (0.40839) | -1 | -1 |
| G: -6257.41721 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.16730 HOMO: -7.00693 LUMO: 2.16331 factor:1 | -1 (0.61560) | -1 | -1 |
| G: -6257.41721 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.30456 HOMO: -6.89537 LUMO: 2.19596 factor:1 | -1 (0.47835) | -1 | -1 |
| G: -6257.41721 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.19543 HOMO: -6.72665 LUMO: 2.03813 factor:1 | 1 (-0.41252) | -1 | -1 |
| G: -6257.41721 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.98688 HOMO: -6.69944 LUMO: 2.36467 factor:1 | 1 (-0.20398) | -1 | -1 |
| G: -6257.41721 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.25317 HOMO: -6.92802 LUMO: 1.72792 factor:1 | 1 (-0.47027) | -1 | -1 |
| G: -6257.41721 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.11018 HOMO: -6.12256 LUMO: 1.85310 factor:1 | 1 (-0.32727) | -1 | -1 |
| G: -6257.41721 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.85153 HOMO: -6.70489 LUMO: 2.20956 factor:1 | 1 (-0.06863) | -1 | -1 |
| G: -6257.41721 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.97635 HOMO: -6.94707 LUMO: 1.81500 factor:1 | 1 (-0.19345) | -1 | -1 |
| G: -6257.41721 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.07845 HOMO: -6.39468 LUMO: 1.79051 factor:1 | 1 (-0.29554) | -1 | -1 |
| G: -6257.41721 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.22100 HOMO: -6.69128 LUMO: 2.03813 factor:1 | 1 (-1.43809) | -1 | -1 |
| G: -6257.41721 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12524.12845 HOMO: -6.55250 LUMO: 2.00548 factor:1 | 1 (-2.34554) | -1 | -1 |
| G: -6257.41721 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12524.18613 HOMO: -6.24773 LUMO: 2.09256 factor:1 | 1 (-2.40323) | -1 | -1 |
| G: -6257.41721 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.70961 HOMO: -6.85727 LUMO: 1.70071 factor:1 | 1 (-1.92670) | -1 | -1 |
| G: -6257.41721 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.96208 HOMO: -6.71305 LUMO: 1.72520 factor:1 | 1 (-1.17918) | -1 | -1 |
| G: -6257.41721 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.15469 HOMO: -6.81101 LUMO: 2.15514 factor:1 | 1 (-1.37178) | -1 | -1 |
| G: -6257.41721 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.34944 HOMO: -6.93618 LUMO: 1.75513 factor:1 | 1 (-1.56653) | -1 | -1 |
| G: -6257.41721 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.57389 HOMO: -6.63686 LUMO: 2.09800 factor:1 | 1 (-0.79098) | -1 | -1 |
| G: -6257.41721 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.28907 HOMO: -6.98244 LUMO: 1.72520 factor:1 | -1 (0.49383) | -1 | -1 |
| G: -6257.41721 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.11597 HOMO: -6.37019 LUMO: 2.35923 factor:1 | 1 (-0.33307) | -1 | -1 |
| G: -6257.41721 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.33824 HOMO: -6.55794 LUMO: 2.12521 factor:1 | 1 (-0.55533) | -1 | -1 |
| G: -6257.41721 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.92623 HOMO: -6.45998 LUMO: 1.93201 factor:1 | 1 (-0.14332) | -1 | -1 |
| G: -6257.41721 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.26936 HOMO: -6.71033 LUMO: 1.58370 factor:1 | 1 (-0.48646) | -1 | -1 |
| G: -6257.41721 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.54926 HOMO: -6.67223 LUMO: 1.52928 factor:1 | 1 (-0.76635) | -1 | -1 |
| G: -6257.41721 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.28270 HOMO: -6.72121 LUMO: 1.33608 factor:1 | 1 (-0.49979) | -1 | -1 |
| G: -6257.41721 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.93959 HOMO: -6.89264 LUMO: 2.08983 factor:1 | 1 (-0.15668) | -1 | -1 |
| G: -6257.41721 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.58608 HOMO: -6.31032 LUMO: 2.24766 factor:1 | 1 (-0.80317) | -1 | -1 |
| G: -6257.41721 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.38948 HOMO: -6.79740 LUMO: 2.09528 factor:1 | 1 (-0.60657) | -1 | -1 |
| G: -6257.41721 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.38616 HOMO: -6.78108 LUMO: 2.15786 factor:1 | 1 (-0.60325) | -1 | -1 |
| G: -6257.41721 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.61239 HOMO: -6.50896 LUMO: 2.15786 factor:1 | 1 (-0.82948) | -1 | -1 |
| G: -6257.41721 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.75329 HOMO: -6.56067 LUMO: 2.24494 factor:1 | 1 (-0.97039) | -1 | -1 |
| G: -6257.41721 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.26011 HOMO: -6.72938 LUMO: 2.24494 factor:1 | 1 (-0.47721) | -1 | -1 |
| G: -6257.41721 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.51138 HOMO: -6.40556 LUMO: 1.58642 factor:1 | 1 (-0.72848) | -1 | -1 |
| G: -6257.41721 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.52638 HOMO: -6.63141 LUMO: 1.66262 factor:1 | 1 (-0.74347) | -1 | -1 |
| G: -6257.41721 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.43054 HOMO: -6.97156 LUMO: 2.23678 factor:1 | 1 (-0.64763) | -1 | -1 |
| G: -6257.41721 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.28116 HOMO: -6.86271 LUMO: 1.91296 factor:1 | -1 (0.50175) | -1 | -1 |
| G: -6257.41721 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12520.93492 HOMO: -6.50624 LUMO: 1.89119 factor:1 | -1 (0.84799) | -1 | -1 |
| G: -6257.41721 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.27778 HOMO: -6.70761 LUMO: 1.56193 factor:1 | -1 (0.50512) | -1 | -1 |
| G: -6257.41721 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.67617 HOMO: -6.60420 LUMO: 1.79595 factor:1 | 1 (-0.89327) | -1 | -1 |
| G: -6257.41721 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.27347 HOMO: -6.85727 LUMO: 2.26943 factor:1 | 1 (-0.49057) | -1 | -1 |
| G: -6257.41721 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.47742 HOMO: -6.23413 LUMO: 1.91024 factor:1 | 1 (-0.69452) | -1 | -1 |
| G: -6257.41721 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.93477 HOMO: -6.84366 LUMO: 2.01364 factor:1 | 1 (-0.15187) | -1 | -1 |
| G: -6257.41721 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.24109 HOMO: -6.63414 LUMO: 2.54971 factor:1 | 1 (-0.45819) | -1 | -1 |
| G: -6257.41721 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.28558 HOMO: -6.52257 LUMO: 2.42998 factor:1 | 1 (-0.50268) | -1 | -1 |
| G: -6257.41721 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.20602 HOMO: -6.61509 LUMO: 2.31297 factor:1 | 1 (-0.42311) | -1 | -1 |
| G: -6257.41721 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.92446 HOMO: -6.45998 LUMO: 2.23405 factor:1 | 1 (-0.14155) | -1 | -1 |
| G: -6257.41721 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.02356 HOMO: -6.86271 LUMO: 2.22317 factor:1 | 1 (-0.24066) | -1 | -1 |
| G: -6257.41721 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.74288 HOMO: -6.84366 LUMO: 2.11432 factor:1 | -1 (0.04003) | -1 | -1 |
| G: -6257.41721 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.16985 HOMO: -6.85999 LUMO: 2.44902 factor:1 | 1 (-0.38695) | -1 | -1 |
| G: -6257.41721 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.44227 HOMO: -6.73482 LUMO: 1.93745 factor:1 | -1 (0.34063) | -1 | -1 |
| G: -6257.41721 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.36690 HOMO: -6.91441 LUMO: 2.32385 factor:1 | -1 (0.41601) | -1 | -1 |
| G: -6257.41721 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12520.86376 HOMO: -6.16066 LUMO: 2.26399 factor:1 | -1 (0.91915) | -1 | -1 |
| G: -6257.41721 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.15043 HOMO: -6.71305 LUMO: 2.38644 factor:1 | -1 (0.63247) | -1 | -1 |
| G: -6257.41721 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.47558 HOMO: -7.08312 LUMO: 2.01636 factor:1 | -1 (0.30733) | 1 | 1 |
| G: -6257.41721 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.55945 HOMO: -6.15249 LUMO: 1.90752 factor:1 | -1 (0.22346) | -1 | -1 |
| G: -6257.41721 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.74087 HOMO: -6.83006 LUMO: 2.25855 factor:1 | -1 (0.04204) | -1 | -1 |
| G: -6257.41721 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.91254 HOMO: -6.77836 LUMO: 2.24766 factor:1 | 1 (-0.12964) | -1 | -1 |
| G: -6257.41721 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.39217 HOMO: -6.66951 LUMO: 2.35923 factor:1 | 1 (-0.60926) | -1 | -1 |
| G: -6257.41721 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.45666 HOMO: -6.68312 LUMO: 2.30208 factor:1 | 1 (-0.67375) | -1 | -1 |
| G: -6257.41721 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.02263 HOMO: -6.49808 LUMO: 2.49801 factor:1 | 1 (-1.23972) | -1 | -1 |
| G: -6257.41721 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.02990 HOMO: -6.62325 LUMO: 1.89935 factor:1 | 1 (-1.24699) | -1 | -1 |
| G: -6257.41721 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.24746 HOMO: -6.80829 LUMO: 1.91296 factor:1 | 1 (-0.46455) | -1 | -1 |
| G: -6257.41721 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.79479 HOMO: -6.64230 LUMO: 2.13065 factor:1 | 1 (-1.01188) | -1 | -1 |
| G: -6257.41721 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.49862 HOMO: -6.40556 LUMO: 1.83949 factor:1 | 1 (-0.71571) | -1 | -1 |
| G: -6257.41721 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.13491 HOMO: -6.48175 LUMO: 1.72248 factor:1 | 1 (-0.35201) | -1 | -1 |
| G: -6257.41721 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.29655 HOMO: -6.61781 LUMO: 2.11432 factor:1 | 1 (-0.51364) | -1 | -1 |
| G: -6257.41721 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.99883 HOMO: -6.34570 LUMO: 2.22317 factor:1 | 1 (-0.21592) | -1 | -1 |
| G: -6257.41721 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.28585 HOMO: -7.00149 LUMO: 1.80139 factor:1 | 1 (-0.50295) | -1 | -1 |
| G: -6257.41721 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.21506 HOMO: -6.66951 LUMO: 2.13065 factor:1 | -1 (0.56785) | -1 | -1 |
| G: -6257.41721 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.29101 HOMO: -6.54434 LUMO: 2.20140 factor:1 | -1 (0.49190) | -1 | -1 |
| G: -6257.41721 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.22760 HOMO: -6.67767 LUMO: 2.02997 factor:1 | -1 (0.55530) | -1 | -1 |
| G: -6257.41721 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.15109 HOMO: -6.49536 LUMO: 2.42998 factor:1 | -1 (0.63182) | -1 | -1 |
| G: -6257.41721 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.16891 HOMO: -6.70761 LUMO: 2.71025 factor:1 | -1 (0.61400) | -1 | -1 |
| G: -6257.41721 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.05182 HOMO: -6.62869 LUMO: 2.11160 factor:1 | -1 (0.73109) | -1 | -1 |
| G: -6257.41721 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.45805 HOMO: -6.61781 LUMO: 2.24494 factor:1 | 1 (-0.67514) | -1 | -1 |
| G: -6257.41721 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.01395 HOMO: -6.66135 LUMO: 2.20956 factor:1 | 1 (-1.23104) | -1 | -1 |
| G: -6257.41721 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.74042 HOMO: -6.95523 LUMO: 2.03813 factor:1 | 1 (-0.95751) | -1 | -1 |
| G: -6257.41721 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.12012 HOMO: -7.11578 LUMO: 2.41365 factor:1 | -1 (0.66279) | 1 | 1 |
| G: -6257.41721 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.69291 HOMO: -6.99061 LUMO: 2.13881 factor:1 | 1 (-0.91000) | -1 | -1 |
| G: -6257.41721 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.39290 HOMO: -6.43277 LUMO: 2.01364 factor:1 | 1 (-0.61000) | -1 | -1 |
| G: -6257.41721 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.48886 HOMO: -6.79196 LUMO: 2.04358 factor:1 | -1 (0.29405) | -1 | -1 |
| G: -6257.41721 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.54763 HOMO: -7.08584 LUMO: 1.99732 factor:1 | 1 (-0.76472) | 1 | 1 |
| G: -6257.41721 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.78378 HOMO: -6.46815 LUMO: 2.29936 factor:1 | 1 (-0.00087) | -1 | -1 |
| G: -6257.41721 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.11225 HOMO: -6.78108 LUMO: 1.93745 factor:1 | 1 (-0.32934) | -1 | -1 |
| G: -6257.41721 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.15930 HOMO: -6.43277 LUMO: 1.80956 factor:1 | -1 (0.62360) | -1 | -1 |
| G: -6257.41721 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.19441 HOMO: -6.71577 LUMO: -0.81090 factor:1 | -1 (0.58850) | -1 | -1 |
| G: -6257.41721 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.23299 HOMO: -7.14027 LUMO: -0.68028 factor:1 | -1 (0.54991) | -1 | -1 |
| G: -6257.41721 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.31601 HOMO: -7.03414 LUMO: -0.69661 factor:1 | -1 (0.46689) | -1 | -1 |
| G: -6257.41721 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.15661 HOMO: -6.64502 LUMO: -0.47348 factor:1 | -1 (0.62630) | -1 | -1 |
| G: -6257.41721 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.26423 HOMO: -6.60692 LUMO: 2.12793 factor:1 | -1 (0.51868) | -1 | -1 |
| G: -6257.41721 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.38249 HOMO: -6.66407 LUMO: 1.94561 factor:1 | -1 (0.40042) | -1 | -1 |
| G: -6257.41721 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12520.99631 HOMO: -7.10217 LUMO: 1.92384 factor:1 | -1 (0.78660) | 1 | 1 |
| G: -6257.41721 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.27751 HOMO: -6.84094 LUMO: 1.66534 factor:1 | -1 (0.50540) | -1 | -1 |
| G: -6257.41721 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12520.97764 HOMO: -6.93618 LUMO: 2.13065 factor:1 | -1 (0.80527) | -1 | -1 |
| G: -6257.41721 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.18763 HOMO: -6.60692 LUMO: 2.20684 factor:1 | -1 (0.59528) | -1 | -1 |
| G: -6257.41721 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.03413 HOMO: -6.85727 LUMO: 2.19324 factor:1 | -1 (0.74878) | -1 | -1 |
| G: -6257.41721 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.14597 HOMO: -6.31032 LUMO: 1.76330 factor:1 | -1 (0.63694) | -1 | -1 |
| G: -6257.41721 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.32722 HOMO: -6.43821 LUMO: 2.10072 factor:1 | -1 (0.45568) | -1 | -1 |
| G: -6257.41721 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.32118 HOMO: -6.42189 LUMO: 2.19596 factor:1 | -1 (0.46172) | -1 | -1 |
| G: -6257.41721 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.29762 HOMO: -6.40556 LUMO: 2.02181 factor:1 | -1 (0.48529) | -1 | -1 |
| G: -6257.41721 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.35191 HOMO: -6.41372 LUMO: 2.26671 factor:1 | -1 (0.43100) | -1 | -1 |
| G: -6257.41721 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.10613 HOMO: -6.60692 LUMO: 2.09800 factor:1 | -1 (0.67677) | -1 | -1 |
| G: -6257.41721 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12520.99032 HOMO: -6.75931 LUMO: 1.76602 factor:1 | -1 (0.79259) | -1 | -1 |
| G: -6257.41721 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.11903 HOMO: -6.39195 LUMO: 1.84221 factor:1 | -1 (0.66388) | -1 | -1 |
| G: -6257.41721 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.20641 HOMO: -6.74570 LUMO: 2.04085 factor:1 | -1 (0.57650) | -1 | -1 |
| G: -6257.41721 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.23065 HOMO: -6.77019 LUMO: 2.16875 factor:1 | -1 (0.55226) | -1 | -1 |
| G: -6257.41721 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.84772 HOMO: -6.15522 LUMO: 1.81772 factor:1 | 1 (-0.06482) | -1 | -1 |
| G: -6257.41721 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.84225 HOMO: -6.48175 LUMO: 2.02453 factor:1 | 1 (-0.05935) | -1 | -1 |
| G: -6257.41721 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.95804 HOMO: -6.57427 LUMO: 1.77962 factor:1 | 1 (-0.17513) | -1 | -1 |
| G: -6257.41721 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.89110 HOMO: -6.57699 LUMO: 2.42998 factor:1 | 1 (-0.10819) | -1 | -1 |
| G: -6257.41721 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.32540 HOMO: -6.35386 LUMO: 2.25310 factor:1 | -1 (0.45751) | -1 | -1 |
| G: -6257.41721 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.33860 HOMO: -6.80013 LUMO: 2.11160 factor:1 | -1 (0.44431) | -1 | -1 |
| G: -6257.41721 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12520.95103 HOMO: -6.24229 LUMO: 2.05718 factor:1 | -1 (0.83188) | -1 | -1 |
| G: -6257.41721 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.20390 HOMO: -6.42733 LUMO: 1.76874 factor:1 | -1 (0.57900) | -1 | -1 |
| G: -6257.41721 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.66149 HOMO: -6.56883 LUMO: 2.36195 factor:1 | -1 (0.12142) | -1 | -1 |
| G: -6257.41721 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.80655 HOMO: -6.72665 LUMO: 2.28848 factor:1 | 1 (-0.02365) | -1 | -1 |
| G: -6257.41721 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.70359 HOMO: -6.39195 LUMO: 1.79051 factor:1 | -1 (0.07932) | -1 | -1 |
| G: -6257.41721 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12520.71211 HOMO: -6.70761 LUMO: 0.15510 factor:1 | -1 (1.07080) | -1 | -1 |
| G: -6257.41721 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12520.97443 HOMO: -6.44366 LUMO: -0.16871 factor:1 | -1 (0.80848) | -1 | -1 |
| G: -6257.41721 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.19811 HOMO: -6.68584 LUMO: 1.69527 factor:1 | -1 (0.58480) | -1 | -1 |
| G: -6257.41721 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12520.99636 HOMO: -6.26950 LUMO: 1.61636 factor:1 | -1 (0.78655) | -1 | -1 |
| G: -6257.41721 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.41661 HOMO: -6.47631 LUMO: 1.98915 factor:1 | -1 (0.36629) | -1 | -1 |
| G: -6257.41721 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.55313 HOMO: -6.58243 LUMO: 1.97283 factor:1 | -1 (0.22977) | -1 | -1 |
| G: -6257.41721 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.53368 HOMO: -6.51713 LUMO: 1.97283 factor:1 | -1 (0.24923) | -1 | -1 |
| G: -6257.41721 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.49403 HOMO: -6.65046 LUMO: 1.69255 factor:1 | -1 (0.28888) | -1 | -1 |
| G: -6257.41721 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.02609 HOMO: -6.26406 LUMO: 2.21773 factor:1 | 1 (-0.24319) | -1 | -1 |
| G: -6257.41721 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.99331 HOMO: -6.88992 LUMO: 2.28304 factor:1 | 1 (-0.21040) | -1 | -1 |
| G: -6257.41721 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.91513 HOMO: -6.67767 LUMO: 2.34834 factor:1 | 1 (-0.13222) | -1 | -1 |
| G: -6257.41721 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.87646 HOMO: -6.52801 LUMO: 2.10344 factor:1 | 1 (-0.09355) | -1 | -1 |
| G: -6257.41721 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.96890 HOMO: -6.52801 LUMO: 2.24222 factor:1 | 1 (-0.18599) | -1 | -1 |
| G: -6257.41721 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.95948 HOMO: -6.17154 LUMO: 1.89663 factor:1 | 1 (-0.17657) | -1 | -1 |
| G: -6257.41721 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.82661 HOMO: -6.42733 LUMO: 2.15514 factor:1 | 1 (-0.04370) | -1 | -1 |
| G: -6257.41721 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.37893 HOMO: -6.36474 LUMO: 2.01364 factor:1 | -1 (0.40398) | -1 | -1 |
| G: -6257.41721 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.11280 HOMO: -6.82189 LUMO: 1.86942 factor:1 | -1 (0.67011) | -1 | -1 |
| G: -6257.41721 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.23784 HOMO: -6.60148 LUMO: 2.00548 factor:1 | -1 (0.54507) | -1 | -1 |
| G: -6257.41721 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.36646 HOMO: -6.67767 LUMO: 2.15786 factor:1 | -1 (0.41644) | -1 | -1 |
| G: -6257.41721 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.33119 HOMO: -6.79196 LUMO: 2.06534 factor:1 | 1 (-0.54828) | -1 | -1 |
| G: -6257.41721 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.36417 HOMO: -6.70216 LUMO: 1.83405 factor:1 | 1 (-0.58126) | -1 | -1 |
| G: -6257.41721 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.31282 HOMO: -6.58788 LUMO: 1.79051 factor:1 | 1 (-0.52991) | -1 | -1 |
| G: -6257.41721 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.57008 HOMO: -6.34842 LUMO: 1.80139 factor:1 | 1 (-0.78717) | -1 | -1 |
| G: -6257.41721 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.47103 HOMO: -6.48175 LUMO: 1.95922 factor:1 | 1 (-0.68812) | -1 | -1 |
| G: -6257.41721 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.55476 HOMO: -6.71033 LUMO: 2.02997 factor:1 | 1 (-0.77185) | -1 | -1 |
| G: -6257.41721 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.63914 HOMO: -6.89264 LUMO: 2.42726 factor:1 | 1 (-0.85623) | -1 | -1 |
| G: -6257.41721 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.37704 HOMO: -6.74570 LUMO: 2.20684 factor:1 | 1 (-0.59413) | -1 | -1 |
| G: -6257.41721 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.08550 HOMO: -6.30216 LUMO: 2.15242 factor:1 | 1 (-0.30259) | -1 | -1 |
| G: -6257.41721 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.04199 HOMO: -6.94979 LUMO: 2.43814 factor:1 | 1 (-0.25908) | -1 | -1 |
| G: -6257.41721 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.15048 HOMO: -6.97972 LUMO: 2.11432 factor:1 | 1 (-0.36757) | -1 | -1 |
| G: -6257.41721 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.82046 HOMO: -6.17154 LUMO: 1.98099 factor:1 | 1 (-0.03755) | -1 | -1 |
| G: -6257.41721 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.96307 HOMO: -6.74026 LUMO: 2.21501 factor:1 | 1 (-0.18017) | -1 | -1 |
| G: -6257.41721 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.06656 HOMO: -6.72393 LUMO: 2.19596 factor:1 | 1 (-0.28365) | -1 | -1 |
| G: -6257.41721 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.98599 HOMO: -6.11440 LUMO: 2.10072 factor:1 | 1 (-0.20308) | -1 | -1 |
| G: -6257.41721 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.81549 HOMO: -6.34297 LUMO: 1.92657 factor:1 | 1 (-2.03258) | -1 | -1 |
| G: -6257.41721 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.10105 HOMO: -6.24773 LUMO: 2.00276 factor:1 | 1 (-1.31815) | -1 | -1 |
| G: -6257.41721 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.81864 HOMO: -6.75114 LUMO: 1.98643 factor:1 | 1 (-2.03574) | -1 | -1 |
| G: -6257.41721 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.14171 HOMO: -6.69128 LUMO: 2.08711 factor:1 | 1 (-1.35880) | -1 | -1 |
| G: -6257.41721 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.10149 HOMO: -6.65318 LUMO: 2.15514 factor:1 | 1 (-1.31858) | -1 | -1 |
| G: -6257.41721 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.67225 HOMO: -6.67495 LUMO: 1.72248 factor:1 | 1 (-1.88934) | -1 | -1 |
| G: -6257.41721 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.23156 HOMO: -6.58243 LUMO: 1.83405 factor:1 | 1 (-1.44865) | -1 | -1 |
| G: -6257.41721 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.33581 HOMO: -6.61237 LUMO: 1.69799 factor:1 | 1 (-1.55290) | -1 | -1 |
| G: -6257.41721 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.61559 HOMO: -6.57427 LUMO: 2.29936 factor:1 | 1 (-1.83269) | -1 | -1 |
| G: -6257.41721 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.99361 HOMO: -6.40012 LUMO: 2.35378 factor:1 | 1 (-2.21071) | -1 | -1 |
| G: -6257.41721 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.12756 HOMO: -6.90081 LUMO: 2.26671 factor:1 | 1 (-1.34465) | -1 | -1 |
| G: -6257.41721 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.05330 HOMO: -6.44910 LUMO: 2.25855 factor:1 | 1 (-1.27039) | -1 | -1 |
| G: -6257.41721 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.46797 HOMO: -6.61509 LUMO: 2.26943 factor:1 | 1 (-1.68507) | -1 | -1 |
| G: -6257.41721 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.11371 HOMO: -6.78924 LUMO: 2.09256 factor:1 | 1 (-1.33080) | -1 | -1 |
| G: -6257.41721 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.67472 HOMO: -6.47087 LUMO: 1.97555 factor:1 | 1 (-1.89182) | -1 | -1 |
| G: -6257.41721 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.15637 HOMO: -6.75931 LUMO: 1.98643 factor:1 | 1 (-1.37347) | -1 | -1 |
| G: -6257.41721 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.18345 HOMO: -6.17971 LUMO: 2.09800 factor:1 | 1 (-1.40054) | -1 | -1 |
| G: -6257.41721 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.15624 HOMO: -6.83006 LUMO: 1.91840 factor:1 | 1 (-1.37333) | -1 | -1 |
| G: -6257.41721 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.96666 HOMO: -6.72938 LUMO: 2.17419 factor:1 | 1 (-1.18375) | -1 | -1 |
| G: -6257.41721 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.79786 HOMO: -6.78924 LUMO: 2.42726 factor:1 | 1 (-1.01496) | -1 | -1 |
| G: -6257.41721 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.06176 HOMO: -6.41372 LUMO: 1.93745 factor:1 | 1 (-1.27885) | -1 | -1 |
| G: -6257.41721 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.28400 HOMO: -6.85455 LUMO: 2.14970 factor:1 | 1 (-1.50109) | -1 | -1 |
| G: -6257.41721 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.24877 HOMO: -6.38651 LUMO: 2.18507 factor:1 | 1 (-0.46586) | -1 | -1 |
| G: -6257.41721 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.42425 HOMO: -6.81373 LUMO: 2.00548 factor:1 | 1 (-0.64135) | -1 | -1 |
| G: -6257.41721 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.85906 HOMO: -6.64774 LUMO: 2.41365 factor:1 | 1 (-1.07616) | -1 | -1 |
| G: -6257.41721 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.93019 HOMO: -6.70489 LUMO: 2.31569 factor:1 | 1 (-1.14729) | -1 | -1 |
| G: -6257.41721 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.93368 HOMO: -6.49264 LUMO: 1.78779 factor:1 | 1 (-1.15077) | -1 | -1 |
| G: -6257.41721 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.91686 HOMO: -6.81101 LUMO: 1.86670 factor:1 | 1 (-1.13395) | -1 | -1 |
| G: -6257.41721 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.55544 HOMO: -6.72121 LUMO: 1.48846 factor:1 | 1 (-0.77253) | -1 | -1 |
| G: -6257.41721 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.83925 HOMO: -6.35930 LUMO: 1.78507 factor:1 | 1 (-1.05635) | -1 | -1 |
| G: -6257.41721 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.86527 HOMO: -6.38651 LUMO: 2.04358 factor:1 | 1 (-1.08236) | -1 | -1 |
| G: -6257.41721 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.73601 HOMO: -6.42189 LUMO: 1.99187 factor:1 | 1 (-0.95311) | -1 | -1 |
| G: -6257.41721 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.34088 HOMO: -6.69400 LUMO: 1.61091 factor:1 | 1 (-0.55797) | -1 | -1 |
| G: -6257.41721 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.33318 HOMO: -6.81101 LUMO: 2.17419 factor:1 | 1 (-0.55027) | -1 | -1 |
| G: -6257.41721 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.16066 HOMO: -6.90897 LUMO: 2.28576 factor:1 | 1 (-0.37775) | -1 | -1 |
| G: -6257.41721 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.15519 HOMO: -6.75387 LUMO: 2.31297 factor:1 | 1 (-0.37228) | -1 | -1 |
| G: -6257.41721 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.31312 HOMO: -7.05863 LUMO: 2.18780 factor:1 | 1 (-0.53021) | -1 | -1 |
| G: -6257.41721 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.26166 HOMO: -6.56611 LUMO: 1.99187 factor:1 | 1 (-0.47876) | -1 | -1 |
| G: -6257.41721 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.08972 HOMO: -6.59060 LUMO: 1.86398 factor:1 | 1 (-0.30681) | -1 | -1 |
| G: -6257.41721 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.24419 HOMO: -6.59060 LUMO: 1.59459 factor:1 | 1 (-0.46129) | -1 | -1 |
| G: -6257.41721 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.38554 HOMO: -6.57699 LUMO: 1.48030 factor:1 | -1 (0.39737) | -1 | -1 |
| G: -6257.41721 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12520.93339 HOMO: -6.99605 LUMO: 2.30208 factor:1 | -1 (0.84951) | -1 | -1 |
| G: -6257.41721 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.09634 HOMO: -6.42189 LUMO: 2.20412 factor:1 | -1 (0.68657) | -1 | -1 |
| G: -6257.41721 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.11035 HOMO: -7.15115 LUMO: 1.83405 factor:1 | -1 (0.67256) | 1 | 1 |
| G: -6257.41721 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12520.98825 HOMO: -7.08040 LUMO: 2.21773 factor:1 | -1 (0.79465) | 1 | 1 |
| G: -6257.41721 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.13435 HOMO: -6.72121 LUMO: 1.89663 factor:1 | -1 (0.64856) | -1 | -1 |
| G: -6257.41721 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.30709 HOMO: -6.25590 LUMO: 1.85037 factor:1 | -1 (0.47582) | -1 | -1 |
| G: -6257.41721 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.08537 HOMO: -6.70489 LUMO: 1.98915 factor:1 | -1 (0.69754) | -1 | -1 |
| G: -6257.41721 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.42297 HOMO: -6.53617 LUMO: 2.08439 factor:1 | 1 (-0.64007) | -1 | -1 |
| G: -6257.41721 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.33984 HOMO: -6.69944 LUMO: 1.98915 factor:1 | 1 (-0.55694) | -1 | -1 |
| G: -6257.41721 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.11976 HOMO: -6.79468 LUMO: 1.96466 factor:1 | 1 (-0.33685) | -1 | -1 |
| G: -6257.41721 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12520.85617 HOMO: -6.79468 LUMO: 1.99459 factor:1 | -1 (0.92674) | -1 | -1 |
| G: -6257.41721 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.04330 HOMO: -6.58788 LUMO: 1.98371 factor:1 | -1 (0.73961) | -1 | -1 |
| G: -6257.41721 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.07617 HOMO: -6.58788 LUMO: 2.16603 factor:1 | -1 (0.70673) | -1 | -1 |
| G: -6257.41721 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.75152 HOMO: -6.56883 LUMO: 1.64085 factor:1 | 1 (-0.96862) | -1 | -1 |
| G: -6257.41721 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.53432 HOMO: -7.19197 LUMO: 2.66127 factor:1 | 1 (-0.75142) | 1 | 1 |
| G: -6257.41721 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.90451 HOMO: -6.48175 LUMO: 2.40004 factor:1 | 1 (-0.12161) | -1 | -1 |
| G: -6257.41721 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.72589 HOMO: -6.18515 LUMO: 2.27759 factor:1 | 1 (-0.94298) | -1 | -1 |
| G: -6257.41721 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.01573 HOMO: -6.64774 LUMO: 2.13337 factor:1 | 1 (-0.23282) | -1 | -1 |
| G: -6257.41721 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.05162 HOMO: -6.39740 LUMO: 1.95106 factor:1 | 1 (-0.26871) | -1 | -1 |
| G: -6257.41721 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.17366 HOMO: -6.59332 LUMO: 1.81772 factor:1 | 1 (-0.39076) | -1 | -1 |
| G: -6257.41721 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.03652 HOMO: -6.68312 LUMO: 2.41909 factor:1 | 1 (-0.25361) | -1 | -1 |
| G: -6257.41721 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.98569 HOMO: -5.87494 LUMO: 2.18235 factor:1 | 1 (-0.20278) | -1 | -1 |
| G: -6257.41721 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.02408 HOMO: -6.30488 LUMO: 2.04902 factor:1 | 1 (-0.24117) | -1 | -1 |
| G: -6257.41721 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.98286 HOMO: -6.65046 LUMO: 2.05446 factor:1 | 1 (-0.19995) | -1 | -1 |
| G: -6257.41721 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.94084 HOMO: -6.55794 LUMO: 2.06807 factor:1 | 1 (-0.15793) | -1 | -1 |
| G: -6257.41721 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.99809 HOMO: -6.68040 LUMO: 1.99187 factor:1 | 1 (-0.21519) | -1 | -1 |
| G: -6257.41721 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.48807 HOMO: -6.60965 LUMO: 2.18780 factor:1 | -1 (0.29484) | -1 | -1 |
| G: -6257.41721 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.99883 HOMO: -6.88176 LUMO: 2.10344 factor:1 | 1 (-0.21592) | -1 | -1 |
| G: -6257.41721 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.70652 HOMO: -6.63414 LUMO: 1.70615 factor:1 | -1 (0.07638) | -1 | -1 |
| G: -6257.41721 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.96571 HOMO: -7.15115 LUMO: 2.07351 factor:1 | 1 (-0.18281) | 1 | 1 |
| G: -6257.41721 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.16569 HOMO: -6.85727 LUMO: 2.27759 factor:1 | 1 (-0.38278) | -1 | -1 |
| G: -6257.41721 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.57245 HOMO: -6.91713 LUMO: 2.28848 factor:1 | -1 (0.21045) | -1 | -1 |
| G: -6257.41721 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.00691 HOMO: -7.10217 LUMO: 2.14698 factor:1 | 1 (-0.22400) | 1 | 1 |
| G: -6257.41721 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.05717 HOMO: -6.78108 LUMO: 2.45447 factor:1 | 1 (-0.27426) | -1 | -1 |
| G: -6257.41721 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.74489 HOMO: -6.78380 LUMO: 2.43542 factor:1 | -1 (0.03801) | -1 | -1 |
| G: -6257.41721 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.02057 HOMO: -6.60965 LUMO: 2.33474 factor:1 | 1 (-0.23766) | -1 | -1 |
| G: -6257.41721 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.74764 HOMO: -6.72665 LUMO: 2.25855 factor:1 | -1 (0.03527) | -1 | -1 |
| G: -6257.41721 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.79363 HOMO: -6.27495 LUMO: 2.04358 factor:1 | 1 (-0.01072) | -1 | -1 |
| G: -6257.41721 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.97203 HOMO: -6.17426 LUMO: 1.45853 factor:1 | 1 (-0.18912) | -1 | -1 |
| G: -6257.41721 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.36546 HOMO: -7.21374 LUMO: 2.33474 factor:1 | -1 (0.41745) | 1 | 1 |
| G: -6257.41721 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.02612 HOMO: -6.94707 LUMO: 1.81772 factor:1 | 1 (-0.24322) | -1 | -1 |
| G: -6257.41721 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.56636 HOMO: -6.80829 LUMO: 0.17960 factor:1 | -1 (0.21655) | -1 | -1 |
| G: -6257.41721 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.94832 HOMO: -7.19469 LUMO: 1.60819 factor:1 | 1 (-0.16542) | 1 | 1 |
| G: -6257.41721 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.57482 HOMO: -6.78652 LUMO: 0.53334 factor:1 | -1 (0.20809) | -1 | -1 |
| G: -6257.41721 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.77689 HOMO: -6.70489 LUMO: 0.74559 factor:1 | -1 (0.00601) | -1 | -1 |
| G: -6257.41721 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.88808 HOMO: -6.72393 LUMO: 0.88981 factor:1 | 1 (-0.10517) | -1 | -1 |
| G: -6257.41721 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.91505 HOMO: -4.54430 LUMO: -0.90614 factor:1 | 1 (-0.13214) | -1 | -1 |
| G: -6257.41721 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.83306 HOMO: -6.83006 LUMO: 0.47348 factor:1 | 1 (-0.05015) | -1 | -1 |
| G: -6257.41721 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.94492 HOMO: -7.07496 LUMO: 0.50613 factor:1 | 1 (-0.16202) | -1 | -1 |
| G: -6257.41721 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.36115 HOMO: -6.62053 LUMO: 0.74559 factor:1 | 1 (-0.57824) | -1 | -1 |
| G: -6257.41721 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.31671 HOMO: -6.79196 LUMO: 1.80139 factor:1 | 1 (-0.53381) | -1 | -1 |
| G: -6257.41721 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.30262 HOMO: -6.71033 LUMO: 0.40817 factor:1 | 1 (-0.51971) | -1 | -1 |
| G: -6257.41721 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.40945 HOMO: -6.74026 LUMO: 0.95784 factor:1 | 1 (-0.62654) | -1 | -1 |
| G: -6257.41721 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.17018 HOMO: -7.34707 LUMO: 0.40001 factor:1 | 1 (-0.38727) | -1 | -1 |
| G: -6257.41721 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.85122 HOMO: -6.19875 LUMO: -0.88709 factor:1 | 1 (-2.06831) | -1 | -1 |
| G: -6257.41721 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12524.16431 HOMO: -6.48719 LUMO: -0.14694 factor:1 | 1 (-2.38140) | -1 | -1 |
| G: -6257.41721 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.62114 HOMO: -6.73482 LUMO: -0.01633 factor:1 | 1 (-1.83824) | -1 | -1 |
| G: -6257.41721 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.94599 HOMO: -7.05591 LUMO: -0.20136 factor:1 | 1 (-2.16309) | -1 | -1 |
| G: -6257.41721 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.17431 HOMO: -6.38651 LUMO: -2.07895 factor:1 | 1 (-1.39140) | -1 | -1 |
| G: -6257.41721 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.81530 HOMO: -6.85455 LUMO: -1.03403 factor:1 | 1 (-2.03239) | -1 | -1 |
| G: -6257.41721 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.52131 HOMO: -6.72121 LUMO: -0.99322 factor:1 | 1 (-1.73840) | -1 | -1 |
| G: -6257.41721 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.76513 HOMO: -6.53890 LUMO: -0.10885 factor:1 | 1 (-0.98222) | -1 | -1 |
| G: -6257.41721 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.22299 HOMO: -6.68312 LUMO: 0.21225 factor:1 | 1 (-1.44008) | -1 | -1 |
| G: -6257.41721 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.85802 HOMO: -6.68040 LUMO: 0.21225 factor:1 | 1 (-2.07511) | -1 | -1 |
| G: -6257.41721 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.68275 HOMO: -6.76475 LUMO: -0.64491 factor:1 | 1 (-1.89984) | -1 | -1 |
| G: -6257.41721 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.94641 HOMO: -6.48175 LUMO: 0.41633 factor:1 | 1 (-1.16350) | -1 | -1 |
| G: -6257.41721 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.53161 HOMO: -6.42733 LUMO: 0.16599 factor:1 | -1 (0.25130) | -1 | -1 |
| G: -6257.41721 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.94811 HOMO: -6.66679 LUMO: 0.77825 factor:1 | 1 (-0.16520) | -1 | -1 |
| G: -6257.41721 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.75099 HOMO: -6.75931 LUMO: -0.73471 factor:1 | -1 (0.03192) | -1 | -1 |
| G: -6257.41721 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.88724 HOMO: -6.53617 LUMO: 0.38096 factor:1 | 1 (-0.10433) | -1 | -1 |
| G: -6257.41721 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.91850 HOMO: -6.34297 LUMO: 0.35375 factor:1 | 1 (-0.13559) | -1 | -1 |
| G: -6257.41721 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.78230 HOMO: -7.11850 LUMO: -0.03265 factor:1 | 1 (-0.99939) | -1 | -1 |
| G: -6257.41721 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.47867 HOMO: -5.21914 LUMO: 1.29798 factor:1 | 1 (-0.69577) | -1 | -1 |
| G: -6257.41721 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.47038 HOMO: -7.09129 LUMO: -0.66668 factor:1 | 1 (-0.68747) | -1 | -1 |
| G: -6257.41721 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.90641 HOMO: -6.96884 LUMO: -0.31021 factor:1 | 1 (-1.12350) | -1 | -1 |
| G: -6257.41721 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.66709 HOMO: -6.51713 LUMO: -0.59865 factor:1 | 1 (-0.88418) | -1 | -1 |
| G: -6257.41721 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.61171 HOMO: -6.69400 LUMO: -0.07075 factor:1 | 1 (-0.82880) | -1 | -1 |
| G: -6257.41721 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.79452 HOMO: -5.28173 LUMO: 1.17281 factor:1 | 1 (-1.01161) | -1 | -1 |
| G: -6257.41721 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.61153 HOMO: -6.54434 LUMO: 0.32109 factor:1 | -1 (0.17138) | -1 | -1 |
| G: -6257.41721 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.67482 HOMO: -6.79740 LUMO: -0.24762 factor:1 | -1 (0.10808) | -1 | -1 |
| G: -6257.41721 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.85953 HOMO: -6.91986 LUMO: -0.14694 factor:1 | 1 (-0.07663) | -1 | -1 |
| G: -6257.41721 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.01194 HOMO: -6.75114 LUMO: 0.18504 factor:1 | 1 (-0.22904) | -1 | -1 |
| G: -6257.41721 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.91330 HOMO: -6.74842 LUMO: 0.69389 factor:1 | 1 (-0.13040) | -1 | -1 |
| G: -6257.41721 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.65793 HOMO: -7.01782 LUMO: 0.56600 factor:1 | 1 (-1.87503) | -1 | -1 |
| G: -6257.41721 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.59562 HOMO: -6.47359 LUMO: -0.56600 factor:1 | 1 (-1.81271) | -1 | -1 |
| G: -6257.41721 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.03224 HOMO: -6.63686 LUMO: -0.55783 factor:1 | 1 (-1.24933) | -1 | -1 |
| G: -6257.41721 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.41910 HOMO: -4.13885 LUMO: -2.05446 factor:1 | 1 (-1.63619) | -1 | -1 |
| G: -6257.41721 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.70148 HOMO: -6.34570 LUMO: 0.19864 factor:1 | 1 (-0.91857) | -1 | -1 |
| G: -6257.41721 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.79781 HOMO: -6.47903 LUMO: 0.24762 factor:1 | 1 (-1.01490) | -1 | -1 |
| G: -6257.41721 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.94813 HOMO: -6.15249 LUMO: 0.32109 factor:1 | 1 (-1.16522) | -1 | -1 |
| G: -6257.41721 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.81092 HOMO: -6.84366 LUMO: 0.29116 factor:1 | 1 (-2.02801) | -1 | -1 |
| G: -6257.41721 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.06168 HOMO: -6.34297 LUMO: 0.19864 factor:1 | 1 (-1.27877) | -1 | -1 |
| G: -6257.41721 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.14097 HOMO: -6.51168 LUMO: 0.30749 factor:1 | 1 (-1.35807) | -1 | -1 |
| G: -6257.41721 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.10179 HOMO: -6.79468 LUMO: -0.16599 factor:1 | 1 (-1.31888) | -1 | -1 |
| G: -6257.41721 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.17042 HOMO: -7.24095 LUMO: 0.15238 factor:1 | 1 (-0.38752) | -1 | -1 |
| G: -6257.41721 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.13732 HOMO: -7.06952 LUMO: -0.34558 factor:1 | -1 (0.64559) | -1 | -1 |
| G: -6257.41721 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.50277 HOMO: -6.88176 LUMO: 0.02177 factor:1 | -1 (0.28014) | -1 | -1 |
| G: -6257.41721 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.52027 HOMO: -6.37291 LUMO: -0.69117 factor:1 | 1 (-1.73737) | -1 | -1 |
| G: -6257.41721 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.15556 HOMO: -6.83278 LUMO: -0.59049 factor:1 | 1 (-1.37265) | -1 | -1 |
| G: -6257.41721 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.35782 HOMO: -6.57155 LUMO: -0.33470 factor:1 | 1 (-1.57491) | -1 | -1 |
| G: -6257.41721 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12524.02450 HOMO: -6.89537 LUMO: -0.58504 factor:1 | 1 (-2.24159) | -1 | -1 |
| G: -6257.41721 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12524.15536 HOMO: -6.57155 LUMO: -0.34831 factor:1 | 1 (-2.37245) | -1 | -1 |
| G: -6257.41721 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.31681 HOMO: -6.64774 LUMO: -0.95784 factor:1 | 1 (-1.53391) | -1 | -1 |
| G: -6257.41721 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.37877 HOMO: -6.91713 LUMO: -0.69933 factor:1 | 1 (-1.59587) | -1 | -1 |
| G: -6257.41721 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12524.07528 HOMO: -6.80557 LUMO: -0.65035 factor:1 | 1 (-2.29237) | -1 | -1 |
| G: -6257.41721 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.98181 HOMO: -7.26544 LUMO: -0.79729 factor:1 | 1 (-1.19891) | -1 | -1 |
| G: -6257.41721 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.45835 HOMO: -6.69128 LUMO: -0.16871 factor:1 | 1 (-0.67544) | -1 | -1 |
| G: -6257.41721 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.15839 HOMO: -6.88448 LUMO: 0.13061 factor:1 | 1 (-1.37548) | -1 | -1 |
| G: -6257.41721 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.27725 HOMO: -6.50352 LUMO: 0.12245 factor:1 | 1 (-1.49434) | -1 | -1 |
| G: -6257.41721 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.08313 HOMO: -6.56067 LUMO: 0.17687 factor:1 | 1 (-0.30022) | -1 | -1 |
| G: -6257.41721 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.14830 HOMO: -6.70216 LUMO: 0.25034 factor:1 | 1 (-0.36539) | -1 | -1 |
| G: -6257.41721 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.52787 HOMO: -6.51713 LUMO: -0.78369 factor:1 | 1 (-0.74497) | -1 | -1 |
| G: -6257.41721 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.39146 HOMO: -6.50352 LUMO: 0.12245 factor:1 | 1 (-0.60856) | -1 | -1 |
| G: -6257.41721 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.34571 HOMO: -6.22052 LUMO: -0.83811 factor:1 | 1 (-1.56280) | -1 | -1 |
| G: -6257.41721 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.16693 HOMO: -6.51168 LUMO: -0.76464 factor:1 | 1 (-1.38403) | -1 | -1 |
| G: -6257.41721 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.21494 HOMO: -7.14571 LUMO: -0.80274 factor:1 | 1 (-0.43204) | -1 | -1 |
| G: -6257.41721 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.09570 HOMO: -6.66679 LUMO: -0.88709 factor:1 | 1 (-0.31279) | -1 | -1 |
| G: -6257.41721 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.59313 HOMO: -6.76203 LUMO: -1.43948 factor:1 | 1 (-0.81022) | -1 | -1 |
| G: -6257.41721 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.99498 HOMO: -6.57427 LUMO: -1.62996 factor:1 | 1 (-1.21208) | -1 | -1 |
| G: -6257.41721 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.00913 HOMO: -5.05043 LUMO: 1.24900 factor:1 | 1 (-1.22623) | -1 | -1 |
| G: -6257.41721 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.96471 HOMO: -6.53345 LUMO: 0.23130 factor:1 | 1 (-0.18180) | -1 | -1 |
| G: -6257.41721 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.94299 HOMO: -7.18381 LUMO: -0.22585 factor:1 | 1 (-0.16008) | -1 | -1 |
| G: -6257.41721 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.22400 HOMO: -7.00965 LUMO: -1.79595 factor:1 | 1 (-0.44110) | -1 | -1 |
| G: -6257.41721 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.21015 HOMO: -6.08174 LUMO: -0.82995 factor:1 | 1 (-0.42725) | -1 | -1 |
| G: -6257.41721 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.64408 HOMO: -6.42189 LUMO: -0.84355 factor:1 | 1 (-1.86118) | -1 | -1 |
| G: -6257.41721 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12524.37887 HOMO: -6.53890 LUMO: 0.60409 factor:1 | 1 (-2.59597) | -1 | -1 |
| G: -6257.41721 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.28065 HOMO: -6.62869 LUMO: 0.43810 factor:1 | 1 (-1.49774) | -1 | -1 |
| G: -6257.41721 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.07556 HOMO: -6.68312 LUMO: 0.64491 factor:1 | 1 (-1.29265) | -1 | -1 |
| G: -6257.41721 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.95107 HOMO: -6.42189 LUMO: 1.51295 factor:1 | 1 (-0.16817) | -1 | -1 |
| G: -6257.41721 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.58526 HOMO: -6.17971 LUMO: 1.67622 factor:1 | 1 (-0.80235) | -1 | -1 |
| G: -6257.41721 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.30224 HOMO: -6.79196 LUMO: 1.36873 factor:1 | 1 (-0.51933) | -1 | -1 |
| G: -6257.41721 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.97409 HOMO: -7.38517 LUMO: 0.56328 factor:1 | 1 (-1.19118) | 1 | 1 |
| G: -6257.41721 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.82273 HOMO: -7.56204 LUMO: 0.71566 factor:1 | 1 (-2.03982) | 1 | 1 |
| G: -6257.41721 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12524.02009 HOMO: -6.45726 LUMO: -1.91840 factor:1 | 1 (-2.23718) | -1 | -1 |
| G: -6257.41721 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12524.11304 HOMO: -6.13073 LUMO: -0.97417 factor:1 | 1 (-2.33014) | -1 | -1 |
| G: -6257.41721 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.06726 HOMO: -6.50352 LUMO: -0.69661 factor:1 | 1 (-1.28435) | -1 | -1 |
| G: -6257.41721 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.33668 HOMO: -6.76747 LUMO: -1.71976 factor:1 | 1 (-1.55377) | -1 | -1 |
| G: -6257.41721 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.02990 HOMO: -6.48447 LUMO: -0.89525 factor:1 | 1 (-1.24699) | -1 | -1 |
| G: -6257.41721 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.25020 HOMO: -7.11850 LUMO: -0.71566 factor:1 | 1 (-1.46729) | -1 | -1 |
| G: -6257.41721 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.88233 HOMO: -6.80285 LUMO: -0.49253 factor:1 | 1 (-1.09942) | -1 | -1 |
| G: -6257.41721 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.80674 HOMO: -6.80557 LUMO: -0.88165 factor:1 | 1 (-1.02383) | -1 | -1 |
| G: -6257.41721 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.04570 HOMO: -6.94162 LUMO: -0.08980 factor:1 | -1 (0.73721) | -1 | -1 |
| G: -6257.41721 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.18121 HOMO: -6.97972 LUMO: -0.29388 factor:1 | -1 (0.60170) | -1 | -1 |
| G: -6257.41721 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.05454 HOMO: -6.75114 LUMO: 0.04626 factor:1 | -1 (0.72837) | -1 | -1 |
| G: -6257.41721 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.30140 HOMO: -7.15932 LUMO: 0.68845 factor:1 | -1 (0.48151) | 1 | 1 |
| G: -6257.41721 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.03896 HOMO: -7.36612 LUMO: 0.63675 factor:1 | 1 (-1.25605) | 1 | 1 |
| G: -6257.41721 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.23322 HOMO: -7.02598 LUMO: -0.66124 factor:1 | 1 (-1.45031) | -1 | -1 |
| G: -6257.41721 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.92611 HOMO: -6.89264 LUMO: -0.54967 factor:1 | 1 (-1.14320) | -1 | -1 |
| G: -6257.41721 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.88059 HOMO: -6.97700 LUMO: 0.27756 factor:1 | 1 (-1.09768) | -1 | -1 |
| G: -6257.41721 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.01141 HOMO: -6.60965 LUMO: 0.08163 factor:1 | -1 (0.77150) | -1 | -1 |
| G: -6257.41721 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.15441 HOMO: -6.70761 LUMO: 0.40001 factor:1 | -1 (0.62850) | -1 | -1 |
| G: -6257.41721 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.27186 HOMO: -6.69128 LUMO: 0.23674 factor:1 | 1 (-1.48895) | -1 | -1 |
| G: -6257.41721 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.21145 HOMO: -6.69128 LUMO: -0.69933 factor:1 | 1 (-1.42854) | -1 | -1 |
| G: -6257.41721 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.11469 HOMO: -6.18515 LUMO: -0.85988 factor:1 | 1 (-1.33178) | -1 | -1 |
| G: -6257.41721 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.83855 HOMO: -6.86815 LUMO: -1.90208 factor:1 | 1 (-0.05565) | -1 | -1 |
| G: -6257.41721 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.70889 HOMO: -6.37563 LUMO: -1.74697 factor:1 | -1 (0.07401) | -1 | -1 |
| G: -6257.41721 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.89654 HOMO: -6.75659 LUMO: 0.36463 factor:1 | 1 (-0.11363) | -1 | -1 |
| G: -6257.41721 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.57785 HOMO: -6.91441 LUMO: -0.88981 factor:1 | 1 (-1.79494) | -1 | -1 |
| G: -6257.41721 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.90206 HOMO: -6.71305 LUMO: -0.29933 factor:1 | 1 (-1.11915) | -1 | -1 |
| G: -6257.41721 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.75936 HOMO: -6.91441 LUMO: -1.04492 factor:1 | 1 (-0.97645) | -1 | -1 |
| G: -6257.41721 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.89466 HOMO: -6.05453 LUMO: -0.83539 factor:1 | 1 (-1.11175) | -1 | -1 |
| G: -6257.41721 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12520.10557 HOMO: -7.35252 LUMO: -0.45715 factor:1 | -1 (1.67734) | -1 | -1 |
| G: -6257.41721 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12520.36568 HOMO: -6.41644 LUMO: -0.97417 factor:1 | -1 (1.41722) | -1 | -1 |
| G: -6257.41721 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12520.64373 HOMO: -6.78924 LUMO: 0.36735 factor:1 | -1 (1.13918) | -1 | -1 |
| G: -6257.41721 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12520.79271 HOMO: -6.74298 LUMO: 0.51974 factor:1 | -1 (0.99020) | -1 | -1 |
| G: -6257.41721 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.46887 HOMO: -6.48992 LUMO: 1.44765 factor:1 | 1 (-1.68596) | -1 | -1 |
| G: -6257.41721 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.25186 HOMO: -6.12528 LUMO: 1.57826 factor:1 | 1 (-1.46895) | -1 | -1 |
| G: -6257.41721 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.49655 HOMO: -6.62325 LUMO: 1.57826 factor:1 | 1 (-0.71365) | -1 | -1 |
| G: -6257.41721 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.72434 HOMO: -6.19875 LUMO: 1.29798 factor:1 | 1 (-0.94143) | -1 | -1 |
| G: -6257.41721 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.17061 HOMO: -6.74570 LUMO: 1.52112 factor:1 | 1 (-0.38771) | -1 | -1 |
| G: -6257.41721 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.99692 HOMO: -6.84094 LUMO: 1.48574 factor:1 | 1 (-0.21402) | -1 | -1 |
| G: -6257.41721 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.05535 HOMO: -6.85183 LUMO: 0.33470 factor:1 | 1 (-0.27244) | -1 | -1 |
| G: -6257.41721 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.18830 HOMO: -6.51168 LUMO: 0.48164 factor:1 | 1 (-0.40540) | -1 | -1 |
| G: -6257.41721 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12520.99957 HOMO: -6.25046 LUMO: 0.75648 factor:1 | -1 (0.78333) | -1 | -1 |
| G: -6257.41721 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.26975 HOMO: -6.65591 LUMO: 0.32109 factor:1 | -1 (0.51315) | -1 | -1 |
| G: -6257.41721 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.23088 HOMO: -6.71033 LUMO: 0.40817 factor:1 | 1 (-1.44797) | -1 | -1 |
| G: -6257.41721 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.46009 HOMO: -6.75114 LUMO: 0.73471 factor:1 | 1 (-0.67718) | -1 | -1 |
| G: -6257.41721 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.33630 HOMO: -6.50624 LUMO: 0.59321 factor:1 | 1 (-1.55339) | -1 | -1 |
| G: -6257.41721 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.18535 HOMO: -6.39740 LUMO: 0.83267 factor:1 | 1 (-1.40245) | -1 | -1 |
| G: -6257.41721 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.00753 HOMO: -6.44094 LUMO: 0.65579 factor:1 | 1 (-1.22462) | -1 | -1 |
| G: -6257.41721 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.23905 HOMO: -6.52257 LUMO: 0.05714 factor:1 | 1 (-0.45614) | -1 | -1 |
| G: -6257.41721 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.37549 HOMO: -7.10217 LUMO: 0.49797 factor:1 | 1 (-0.59258) | -1 | -1 |
| G: -6257.41721 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.57008 HOMO: -6.83006 LUMO: 0.55783 factor:1 | 1 (-0.78717) | -1 | -1 |
| G: -6257.41721 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.42923 HOMO: -6.99333 LUMO: -0.79457 factor:1 | 1 (-0.64632) | -1 | -1 |
| G: -6257.41721 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.17105 HOMO: -6.64230 LUMO: 0.32382 factor:1 | 1 (-0.38814) | -1 | -1 |
| G: -6257.41721 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12520.83919 HOMO: -6.90897 LUMO: 0.30749 factor:1 | -1 (0.94372) | -1 | -1 |
| G: -6257.41721 HOMO: -7.26544 LUMO: -1.10478 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.02872 HOMO: -7.09129 LUMO: 1.33336 factor:1 | -1 (0.75419) | 1 | 1 |
| G: -6257.41721 HOMO: -7.26544 LUMO: -1.10478 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.31766 HOMO: -6.66951 LUMO: 1.34424 factor:1 | 1 (-0.53476) | -1 | -1 |
| G: -6257.41721 HOMO: -7.26544 LUMO: -1.10478 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.14944 HOMO: -7.02870 LUMO: 1.48574 factor:1 | 1 (-0.36654) | -1 | -1 |
| G: -6257.41721 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.03649 HOMO: -7.26544 LUMO: 0.32926 factor:1 | 1 (-0.25358) | -1 | -1 |
| G: -6257.41721 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.99426 HOMO: -6.56067 LUMO: -0.45987 factor:1 | 1 (-0.21135) | -1 | -1 |
| G: -6257.41721 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.20757 HOMO: -6.54434 LUMO: -0.28300 factor:1 | 1 (-0.42466) | -1 | -1 |
| G: -6257.41721 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.45184 HOMO: -7.19469 LUMO: 0.54695 factor:1 | 1 (-0.66894) | -1 | -1 |
| G: -6257.41721 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.86383 HOMO: -6.47359 LUMO: -0.22041 factor:1 | 1 (-0.08093) | -1 | -1 |
| G: -6257.41721 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.62641 HOMO: -6.80013 LUMO: 2.08167 factor:1 | 1 (-0.84350) | -1 | -1 |
| G: -6257.41721 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.04136 HOMO: -6.23957 LUMO: 1.67894 factor:1 | 1 (-0.25845) | -1 | -1 |
| G: -6257.41721 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.89396 HOMO: -6.75114 LUMO: -0.62858 factor:1 | 1 (-0.11105) | -1 | -1 |
| G: -6257.41721 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.87956 HOMO: -6.79468 LUMO: -0.64491 factor:1 | 1 (-0.09665) | -1 | -1 |
| G: -6257.41721 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.74685 HOMO: -6.84911 LUMO: -0.69661 factor:1 | -1 (0.03606) | -1 | -1 |
| G: -6257.41721 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.11048 HOMO: -7.54028 LUMO: 0.25851 factor:1 | 1 (-0.32757) | -1 | -1 |
| G: -6257.41721 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.92008 HOMO: -6.92802 LUMO: -0.71022 factor:1 | 1 (-0.13717) | -1 | -1 |
| G: -6257.41721 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12520.29246 HOMO: -6.72665 LUMO: -0.46804 factor:1 | -1 (1.49045) | -1 | -1 |
| G: -6257.41721 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12520.59088 HOMO: -6.63686 LUMO: -0.23674 factor:1 | -1 (1.19202) | -1 | -1 |
| G: -6257.41721 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12520.75350 HOMO: -7.21102 LUMO: 0.54423 factor:1 | -1 (1.02941) | -1 | -1 |
| G: -6257.41721 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.05816 HOMO: -6.63414 LUMO: -0.25034 factor:1 | -1 (0.72475) | -1 | -1 |
| G: -6257.41721 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.08387 HOMO: -6.70761 LUMO: -0.31837 factor:1 | -1 (0.69903) | -1 | -1 |
| G: -6257.41721 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.34791 HOMO: -6.57155 LUMO: 1.76874 factor:1 | -1 (0.43500) | -1 | -1 |
| G: -6257.41721 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.09821 HOMO: -6.84366 LUMO: 2.04358 factor:1 | -1 (0.68469) | -1 | -1 |
| G: -6257.41721 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.37014 HOMO: -6.60420 LUMO: 1.80139 factor:1 | -1 (0.41277) | -1 | -1 |
| G: -6257.41721 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.44614 HOMO: -7.03686 LUMO: 2.21229 factor:1 | -1 (0.33677) | -1 | -1 |
| G: -6257.41721 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.67820 HOMO: -6.77564 LUMO: 1.97555 factor:1 | -1 (0.10471) | -1 | -1 |
| G: -6257.41721 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.69325 HOMO: -6.40012 LUMO: 2.17691 factor:1 | -1 (0.08966) | -1 | -1 |
| G: -6257.41721 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.92819 HOMO: -6.80013 LUMO: 2.25582 factor:1 | 1 (-0.14528) | -1 | -1 |
| G: -6257.41721 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12520.80697 HOMO: -6.74298 LUMO: 2.31569 factor:1 | -1 (0.97594) | -1 | -1 |
| G: -6257.41721 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12520.70365 HOMO: -6.68856 LUMO: 1.85854 factor:1 | -1 (1.07926) | -1 | -1 |
| G: -6257.41721 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12520.75872 HOMO: -6.17971 LUMO: 1.52928 factor:1 | -1 (1.02418) | -1 | -1 |
| G: -6257.41721 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12520.91021 HOMO: -6.54162 LUMO: 1.91840 factor:1 | -1 (0.87270) | -1 | -1 |
| G: -6257.41721 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.02940 HOMO: -6.80013 LUMO: -0.55511 factor:1 | -1 (0.75351) | -1 | -1 |
| G: -6257.41721 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12520.89122 HOMO: -7.46953 LUMO: 0.28572 factor:1 | -1 (0.89169) | -1 | -1 |
| G: -6257.41721 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.12426 HOMO: -6.61781 LUMO: -0.54967 factor:1 | -1 (0.65865) | -1 | -1 |
| G: -6257.41721 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.97352 HOMO: -6.56339 LUMO: -0.47892 factor:1 | 1 (-0.19062) | -1 | -1 |
| G: -6257.41721 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.86049 HOMO: -6.65591 LUMO: -0.25307 factor:1 | 1 (-0.07758) | -1 | -1 |
| G: -6257.41721 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.10727 HOMO: -6.62869 LUMO: -0.23402 factor:1 | 1 (-0.32436) | -1 | -1 |
| G: -6257.41721 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.37491 HOMO: -6.58243 LUMO: -0.19048 factor:1 | 1 (-1.59200) | -1 | -1 |
| G: -6257.41721 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.27629 HOMO: -7.27632 LUMO: 0.52790 factor:1 | 1 (-1.49339) | -1 | -1 |
| G: -6257.41721 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.42344 HOMO: -7.21102 LUMO: 0.57688 factor:1 | 1 (-0.64053) | -1 | -1 |
| G: -6257.41721 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.08786 HOMO: -6.72393 LUMO: -0.53879 factor:1 | 1 (-1.30495) | -1 | -1 |
| G: -6257.41721 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.24036 HOMO: -7.42054 LUMO: -0.99322 factor:1 | 1 (-0.45745) | -1 | -1 |
| G: -6257.41721 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.50534 HOMO: -6.88992 LUMO: -0.71838 factor:1 | 1 (-0.72244) | -1 | -1 |
| G: -6257.41721 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12520.14429 HOMO: -6.88176 LUMO: -0.61226 factor:1 | -1 (1.63862) | -1 | -1 |
| G: -6257.41721 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12520.01264 HOMO: -7.36340 LUMO: -1.04492 factor:1 | -1 (1.77026) | -1 | -1 |
| G: -6257.41721 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12520.21159 HOMO: -6.65863 LUMO: -0.41906 factor:1 | -1 (1.57132) | -1 | -1 |
| G: -6257.41721 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.13277 HOMO: -7.15115 LUMO: -0.66396 factor:1 | -1 (0.65013) | -1 | -1 |
| G: -6257.41721 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12520.95255 HOMO: -7.10489 LUMO: -0.64491 factor:1 | -1 (0.83036) | -1 | -1 |
| G: -6257.41721 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.16126 HOMO: -7.20285 LUMO: 0.47892 factor:1 | -1 (0.62164) | -1 | -1 |
| G: -6257.41721 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12520.80066 HOMO: -6.55794 LUMO: -0.28844 factor:1 | -1 (0.98225) | -1 | -1 |
| G: -6257.41721 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12520.61755 HOMO: -7.19197 LUMO: -0.69661 factor:1 | -1 (1.16535) | -1 | -1 |
| G: -6257.41721 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12520.84907 HOMO: -6.56883 LUMO: -0.32926 factor:1 | -1 (0.93384) | -1 | -1 |
| G: -6257.41721 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.39076 HOMO: -6.70761 LUMO: 1.95650 factor:1 | -1 (0.39214) | -1 | -1 |
| G: -6257.41721 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.32137 HOMO: -6.60420 LUMO: 1.80684 factor:1 | -1 (0.46153) | -1 | -1 |
| G: -6257.41721 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.55460 HOMO: -6.84094 LUMO: 1.64085 factor:1 | -1 (0.22830) | -1 | -1 |
| G: -6257.41721 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.36911 HOMO: -6.69128 LUMO: 1.90208 factor:1 | 1 (-1.58621) | -1 | -1 |
| G: -6257.41721 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.38422 HOMO: -6.75387 LUMO: 1.70343 factor:1 | 1 (-1.60131) | -1 | -1 |
| G: -6257.41721 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.45623 HOMO: -7.07496 LUMO: 2.10072 factor:1 | 1 (-0.67332) | -1 | -1 |
| G: -6257.41721 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.27794 HOMO: -6.99877 LUMO: 2.24494 factor:1 | 1 (-0.49503) | -1 | -1 |
| G: -6257.41721 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.09567 HOMO: -6.63414 LUMO: 2.17691 factor:1 | 1 (-1.31276) | -1 | -1 |
| G: -6257.41721 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.45756 HOMO: -6.44638 LUMO: 1.78235 factor:1 | 1 (-0.67465) | -1 | -1 |
| G: -6257.41721 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.53059 HOMO: -6.87632 LUMO: 1.84221 factor:1 | 1 (-0.74769) | -1 | -1 |
| G: -6257.41721 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.38134 HOMO: -6.85183 LUMO: 1.68711 factor:1 | 1 (-0.59843) | -1 | -1 |
| G: -6257.41721 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.28365 HOMO: -6.96339 LUMO: 2.26671 factor:1 | 1 (-0.50074) | -1 | -1 |
| G: -6257.41721 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.25554 HOMO: -6.63141 LUMO: 1.96738 factor:1 | 1 (-0.47263) | -1 | -1 |
| G: -6257.41721 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.50651 HOMO: -6.37019 LUMO: 2.23133 factor:1 | 1 (-0.72361) | -1 | -1 |
| G: -6257.41721 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.90781 HOMO: -7.11034 LUMO: 2.32385 factor:1 | 1 (-0.12490) | 1 | 1 |
| G: -6257.41721 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.15015 HOMO: -6.91986 LUMO: 1.65445 factor:1 | 1 (-0.36724) | -1 | -1 |
| G: -6257.41721 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.33560 HOMO: -7.12938 LUMO: 2.28304 factor:1 | 1 (-0.55269) | 1 | 1 |
| G: -6257.41721 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.22896 HOMO: -6.54978 LUMO: 1.92112 factor:1 | 1 (-0.44605) | -1 | -1 |
| G: -6257.41721 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.03801 HOMO: -6.83006 LUMO: 2.48712 factor:1 | 1 (-0.25511) | -1 | -1 |
| G: -6257.41721 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.05872 HOMO: -6.97972 LUMO: 1.96738 factor:1 | 1 (-0.27581) | -1 | -1 |
| G: -6257.41721 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.27976 HOMO: -6.69944 LUMO: 2.06262 factor:1 | 1 (-0.49685) | -1 | -1 |
| G: -6257.41721 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12520.86379 HOMO: -6.76747 LUMO: 2.10888 factor:1 | -1 (0.91912) | -1 | -1 |
| G: -6257.41721 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.14265 HOMO: -6.91169 LUMO: 2.06534 factor:1 | -1 (0.64026) | -1 | -1 |
| G: -6257.41721 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.38501 HOMO: -7.03414 LUMO: 1.93473 factor:1 | 1 (-0.60211) | -1 | -1 |
| G: -6257.41721 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.10787 HOMO: -7.03142 LUMO: 2.52250 factor:1 | 1 (-0.32496) | -1 | -1 |
| G: -6257.41721 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12520.81818 HOMO: -6.34025 LUMO: 2.61229 factor:1 | -1 (0.96473) | -1 | -1 |
| G: -6257.41721 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.07549 HOMO: -6.98788 LUMO: 2.28304 factor:1 | -1 (0.70741) | -1 | -1 |
| G: -6257.41721 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.40327 HOMO: -6.97700 LUMO: 2.53882 factor:1 | 1 (-0.62037) | -1 | -1 |
| G: -6257.41721 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.32507 HOMO: -6.58788 LUMO: 1.94289 factor:1 | 1 (-0.54216) | -1 | -1 |
| G: -6257.41721 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.81493 HOMO: -6.78652 LUMO: 2.13609 factor:1 | 1 (-0.03203) | -1 | -1 |
| G: -6257.41721 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.53266 HOMO: -6.55250 LUMO: 1.82861 factor:1 | 1 (-0.74976) | -1 | -1 |
| G: -6257.41721 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.08729 HOMO: -6.45998 LUMO: 1.75786 factor:1 | 1 (-0.30439) | -1 | -1 |
| G: -6257.41721 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12520.66033 HOMO: -6.78924 LUMO: 2.33746 factor:1 | -1 (1.12258) | -1 | -1 |
| G: -6257.41721 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12520.91783 HOMO: -6.85727 LUMO: 1.76058 factor:1 | -1 (0.86508) | -1 | -1 |
| G: -6257.41721 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12520.73048 HOMO: -6.70489 LUMO: 1.84493 factor:1 | -1 (1.05243) | -1 | -1 |
| G: -6257.41721 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12520.97043 HOMO: -6.71305 LUMO: 1.53472 factor:1 | -1 (0.81248) | -1 | -1 |
| G: -6257.41721 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.46992 HOMO: -6.76747 LUMO: 1.48846 factor:1 | -1 (0.31299) | -1 | -1 |
| G: -6257.41721 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.75706 HOMO: -6.69128 LUMO: 1.95922 factor:1 | -1 (0.02585) | -1 | -1 |
| G: -6257.41721 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12520.84675 HOMO: -6.67495 LUMO: 2.05446 factor:1 | -1 (0.93615) | -1 | -1 |
| G: -6257.41721 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.10099 HOMO: -6.63686 LUMO: 2.25310 factor:1 | -1 (0.68192) | -1 | -1 |
| G: -6257.41721 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12524.34127 HOMO: -6.63958 LUMO: 2.14154 factor:1 | 1 (-2.55836) | -1 | -1 |
| G: -6257.41721 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.98145 HOMO: -6.62597 LUMO: 2.01908 factor:1 | 1 (-2.19854) | -1 | -1 |
| G: -6257.41721 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.31891 HOMO: -7.07768 LUMO: 2.14154 factor:1 | 1 (-1.53600) | -1 | -1 |
| G: -6257.41721 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12524.14771 HOMO: -6.19603 LUMO: 2.01092 factor:1 | 1 (-2.36481) | -1 | -1 |
| G: -6257.41721 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.76460 HOMO: -6.65046 LUMO: 2.15786 factor:1 | 1 (-1.98170) | -1 | -1 |
| G: -6257.41721 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.81716 HOMO: -6.92258 LUMO: 2.31841 factor:1 | 1 (-1.03425) | -1 | -1 |
| G: -6257.41721 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.68678 HOMO: -6.90081 LUMO: 2.19324 factor:1 | 1 (-1.90387) | -1 | -1 |
| G: -6257.41721 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.61774 HOMO: -6.85455 LUMO: 1.95650 factor:1 | 1 (-1.83484) | -1 | -1 |
| G: -6257.41721 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.02971 HOMO: -6.57699 LUMO: 1.76058 factor:1 | 1 (-1.24680) | -1 | -1 |
| G: -6257.41721 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.90327 HOMO: -6.90625 LUMO: 1.97555 factor:1 | 1 (-2.12037) | -1 | -1 |
| G: -6257.41721 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.77100 HOMO: -6.97428 LUMO: 1.92929 factor:1 | 1 (-1.98809) | -1 | -1 |
| G: -6257.41721 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12520.88629 HOMO: -6.61781 LUMO: -0.41906 factor:1 | -1 (0.89662) | -1 | -1 |
| G: -6257.41721 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.13128 HOMO: -6.62869 LUMO: -0.81906 factor:1 | -1 (0.65163) | -1 | -1 |
| G: -6257.41721 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.98792 HOMO: -7.01237 LUMO: 2.00548 factor:1 | 1 (-0.20501) | -1 | -1 |
| G: -6257.41721 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.78190 HOMO: -6.85727 LUMO: 2.17691 factor:1 | -1 (0.00101) | -1 | -1 |
| G: -6257.41721 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.75093 HOMO: -6.71849 LUMO: 1.58914 factor:1 | -1 (0.03197) | -1 | -1 |
| G: -6257.41721 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.88136 HOMO: -7.52395 LUMO: 0.27211 factor:1 | 1 (-0.09845) | -1 | -1 |
| G: -6257.41721 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.01156 HOMO: -6.96611 LUMO: -0.72654 factor:1 | 1 (-0.22866) | -1 | -1 |
| G: -6257.41721 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.94299 HOMO: -6.89537 LUMO: -0.68028 factor:1 | 1 (-0.16008) | -1 | -1 |
| G: -6257.41721 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.67063 HOMO: -6.84911 LUMO: -0.58504 factor:1 | -1 (0.11227) | -1 | -1 |
| G: -6257.41721 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.89306 HOMO: -6.79196 LUMO: -0.55783 factor:1 | 1 (-0.11015) | -1 | -1 |
| G: -6257.41721 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.84828 HOMO: -6.67767 LUMO: 1.79323 factor:1 | 1 (-2.06537) | -1 | -1 |
| G: -6257.41721 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.68161 HOMO: -6.54434 LUMO: 1.91024 factor:1 | 1 (-1.89870) | -1 | -1 |
| G: -6257.41721 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.79746 HOMO: -6.62869 LUMO: 1.69799 factor:1 | 1 (-1.01455) | -1 | -1 |
| G: -6257.41721 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.15145 HOMO: -6.72393 LUMO: 2.12249 factor:1 | 1 (-1.36854) | -1 | -1 |
| G: -6257.41721 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.52256 HOMO: -6.66407 LUMO: 2.05990 factor:1 | 1 (-1.73965) | -1 | -1 |
| G: -6257.41721 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.76129 HOMO: -7.00149 LUMO: 1.82044 factor:1 | 1 (-0.97839) | -1 | -1 |
| G: -6257.41721 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.77384 HOMO: -7.12122 LUMO: 2.16058 factor:1 | 1 (-0.99093) | 1 | 1 |
| G: -6257.41721 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.81040 HOMO: -6.63141 LUMO: 2.21229 factor:1 | 1 (-2.02749) | -1 | -1 |
| G: -6257.41721 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.94413 HOMO: -6.37835 LUMO: 2.32113 factor:1 | 1 (-1.16122) | -1 | -1 |
| G: -6257.41721 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.03934 HOMO: -6.99605 LUMO: 2.00548 factor:1 | 1 (-1.25643) | -1 | -1 |
| G: -6257.41721 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.51037 HOMO: -6.85999 LUMO: 2.39460 factor:1 | 1 (-1.72746) | -1 | -1 |
| G: -6257.41721 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12524.12788 HOMO: -6.85727 LUMO: 2.48712 factor:1 | 1 (-2.34497) | -1 | -1 |
| G: -6257.41721 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.28857 HOMO: -7.04231 LUMO: 2.40277 factor:1 | 1 (-1.50566) | -1 | -1 |
| G: -6257.41721 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.30386 HOMO: -6.60692 LUMO: 2.26671 factor:1 | 1 (-1.52095) | -1 | -1 |
| G: -6257.41721 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.96102 HOMO: -6.67495 LUMO: 2.14698 factor:1 | 1 (-1.17812) | -1 | -1 |
| G: -6257.41721 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.00833 HOMO: -6.73210 LUMO: 2.06807 factor:1 | 1 (-0.22542) | -1 | -1 |
| G: -6257.41721 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.97325 HOMO: -7.20013 LUMO: 2.02181 factor:1 | 1 (-0.19034) | 1 | 1 |
| G: -6257.41721 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.24030 HOMO: -7.18653 LUMO: 2.29936 factor:1 | 1 (-0.45740) | 1 | 1 |
| G: -6257.41721 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.18701 HOMO: -6.92802 LUMO: 2.36195 factor:1 | 1 (-1.40411) | -1 | -1 |
| G: -6257.41721 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12524.05171 HOMO: -6.89537 LUMO: 1.78779 factor:1 | 1 (-2.26880) | -1 | -1 |
| G: -6257.41721 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.99575 HOMO: -6.96067 LUMO: 2.31297 factor:1 | 1 (-1.21284) | -1 | -1 |
| G: -6257.41721 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.07961 HOMO: -6.91441 LUMO: 2.50345 factor:1 | 1 (-1.29670) | -1 | -1 |
| G: -6257.41721 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.27502 HOMO: -7.17292 LUMO: 2.12521 factor:1 | 1 (-1.49211) | 1 | 1 |
| G: -6257.41721 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.82293 HOMO: -6.93618 LUMO: 2.35106 factor:1 | 1 (-1.04002) | -1 | -1 |
| G: -6257.41721 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.90540 HOMO: -6.75931 LUMO: 1.61908 factor:1 | 1 (-1.12250) | -1 | -1 |
| G: -6257.41721 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.65819 HOMO: -6.35930 LUMO: 1.23540 factor:1 | 1 (-0.87528) | -1 | -1 |
| G: -6257.41721 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.93803 HOMO: -6.17971 LUMO: 1.84493 factor:1 | 1 (-1.15512) | -1 | -1 |
| G: -6257.41721 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12520.94670 HOMO: -6.72665 LUMO: 2.61229 factor:1 | -1 (0.83621) | -1 | -1 |
| G: -6257.41721 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.98092 HOMO: -6.62869 LUMO: 2.28304 factor:1 | 1 (-0.19802) | -1 | -1 |
| G: -6257.41721 HOMO: -8.88180 LUMO: 1.02315 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.92179 HOMO: -6.58243 LUMO: 0.28028 factor:1 | 1 (-0.13889) | -1 | -1 |
| G: -6257.41721 HOMO: -8.88180 LUMO: 1.02315 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.12169 HOMO: -6.79468 LUMO: 0.14966 factor:1 | 1 (-0.33878) | -1 | -1 |
| G: -6257.41721 HOMO: -8.88180 LUMO: 1.02315 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.09069 HOMO: -6.63141 LUMO: 0.31021 factor:1 | 1 (-0.30779) | -1 | -1 |
| G: -6257.41721 HOMO: -8.88180 LUMO: 1.02315 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12520.69178 HOMO: -6.81101 LUMO: 0.13878 factor:1 | -1 (1.09112) | -1 | -1 |
| G: -6257.41721 HOMO: -8.88180 LUMO: 1.02315 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12520.09286 HOMO: -6.72665 LUMO: 0.65579 factor:1 | -1 (1.69004) | -1 | -1 |
| G: -6257.41721 HOMO: -8.88180 LUMO: 1.02315 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12520.62977 HOMO: -6.53073 LUMO: 0.91430 factor:1 | -1 (1.15314) | -1 | -1 |
| G: -6257.41721 HOMO: -8.88180 LUMO: 1.02315 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.24198 HOMO: -7.19197 LUMO: 1.62996 factor:1 | 1 (-1.45907) | 1 | 1 |
| G: -6257.41721 HOMO: -8.88180 LUMO: 1.02315 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.14054 HOMO: -6.69400 LUMO: 0.84627 factor:1 | 1 (-1.35763) | -1 | -1 |
| G: -6257.41721 HOMO: -8.88180 LUMO: 1.02315 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.34397 HOMO: -6.76475 LUMO: 0.51974 factor:1 | 1 (-1.56106) | -1 | -1 |
| G: -6257.41721 HOMO: -8.88180 LUMO: 1.02315 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.41889 HOMO: -6.67767 LUMO: 0.52246 factor:1 | 1 (-0.63598) | -1 | -1 |
| G: -6257.41721 HOMO: -8.88180 LUMO: 1.02315 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.94424 HOMO: -6.73210 LUMO: 0.94424 factor:1 | 1 (-0.16134) | -1 | -1 |
| G: -6257.41721 HOMO: -8.88180 LUMO: 1.02315 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.86000 HOMO: -6.97972 LUMO: 0.60409 factor:1 | 1 (-0.07709) | -1 | -1 |
| G: -6257.41721 HOMO: -8.88180 LUMO: 1.02315 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.07510 HOMO: -7.38517 LUMO: 0.73743 factor:1 | 1 (-0.29220) | -1 | -1 |
| G: -6257.41721 HOMO: -8.88180 LUMO: 1.02315 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.02215 HOMO: -6.48992 LUMO: 1.08301 factor:1 | 1 (-0.23924) | -1 | -1 |
| G: -6257.41721 HOMO: -8.88180 LUMO: 1.02315 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12520.88988 HOMO: -7.18381 LUMO: 1.61908 factor:1 | -1 (0.89302) | 1 | 1 |
| G: -6257.41721 HOMO: -8.88180 LUMO: 1.02315 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.05395 HOMO: -6.74842 LUMO: 0.57960 factor:1 | 1 (-1.27104) | -1 | -1 |
| G: -6257.41721 HOMO: -8.88180 LUMO: 1.02315 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.14029 HOMO: -6.67495 LUMO: 0.77280 factor:1 | 1 (-1.35739) | -1 | -1 |
| G: -6257.41721 HOMO: -8.88180 LUMO: 1.02315 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.19355 HOMO: -6.74570 LUMO: 0.77280 factor:1 | 1 (-0.41065) | -1 | -1 |
| G: -6257.41721 HOMO: -8.88180 LUMO: 1.02315 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.99779 HOMO: -6.73754 LUMO: 0.86804 factor:1 | 1 (-1.21488) | -1 | -1 |
| G: -6257.41721 HOMO: -8.88180 LUMO: 1.02315 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.11897 HOMO: -6.66135 LUMO: 0.94424 factor:1 | 1 (-0.33606) | -1 | -1 |
| G: -6257.41721 HOMO: -8.88180 LUMO: 1.02315 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.18685 HOMO: -6.44638 LUMO: 1.00138 factor:1 | 1 (-1.40394) | -1 | -1 |
| G: -6257.41721 HOMO: -8.88180 LUMO: 1.02315 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.31968 HOMO: -6.65591 LUMO: 1.02043 factor:1 | 1 (-0.53677) | -1 | -1 |
| G: -6257.41721 HOMO: -8.88180 LUMO: 1.02315 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.33777 HOMO: -7.17564 LUMO: 0.50069 factor:1 | 1 (-0.55487) | -1 | -1 |
| G: -6257.41721 HOMO: -8.88180 LUMO: 1.02315 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.41903 HOMO: -6.59332 LUMO: 0.79457 factor:1 | 1 (-0.63612) | -1 | -1 |
| G: -6257.41721 HOMO: -8.88180 LUMO: 1.02315 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.09549 HOMO: -6.76747 LUMO: 1.73881 factor:1 | -1 (0.68741) | -1 | -1 |
| G: -6257.41721 HOMO: -8.88180 LUMO: 1.02315 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.74199 HOMO: -7.00421 LUMO: 1.07485 factor:1 | 1 (-1.95908) | -1 | -1 |
| G: -6257.41721 HOMO: -8.88180 LUMO: 1.02315 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.86366 HOMO: -6.94979 LUMO: 1.67894 factor:1 | 1 (-1.08075) | -1 | -1 |
| G: -6257.41721 HOMO: -8.88180 LUMO: 1.02315 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.04625 HOMO: -6.66135 LUMO: 0.47076 factor:1 | 1 (-1.26334) | -1 | -1 |
| G: -6257.41721 HOMO: -8.88180 LUMO: 1.02315 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.90731 HOMO: -6.74298 LUMO: 1.85037 factor:1 | 1 (-1.12440) | -1 | -1 |
| G: -6257.41721 HOMO: -8.88180 LUMO: 1.02315 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.10924 HOMO: -6.65318 LUMO: 0.95240 factor:1 | 1 (-1.32634) | -1 | -1 |
| G: -6257.41721 HOMO: -8.88180 LUMO: 1.02315 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.01285 HOMO: -6.63958 LUMO: 0.78097 factor:1 | -1 (0.77006) | -1 | -1 |
| G: -6257.17264 HOMO: -8.88180 LUMO: 1.02315 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.83319 HOMO: -6.11712 LUMO: 0.40001 factor:1 | 1 (-0.29486) | -1 | -1 |
| G: -6257.17264 HOMO: -8.88180 LUMO: 1.02315 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.90577 HOMO: -7.08312 LUMO: 0.92519 factor:1 | 1 (-0.36744) | -1 | -1 |
| G: -6257.17264 HOMO: -8.88180 LUMO: 1.02315 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12520.81143 HOMO: -6.96067 LUMO: 0.54695 factor:1 | -1 (0.72690) | -1 | -1 |
| G: -6257.17264 HOMO: -8.88180 LUMO: 1.02315 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12520.76632 HOMO: -6.74026 LUMO: 0.60137 factor:1 | -1 (0.77201) | -1 | -1 |
| G: -6257.17264 HOMO: -8.88180 LUMO: 1.02315 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12520.79222 HOMO: -6.74298 LUMO: 0.59593 factor:1 | -1 (0.74611) | -1 | -1 |
| G: -6257.17264 HOMO: -8.88180 LUMO: 1.02315 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.52764 HOMO: -6.93074 LUMO: 0.60681 factor:1 | -1 (0.01069) | -1 | -1 |
| G: -6257.17264 HOMO: -8.88180 LUMO: 1.02315 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.26042 HOMO: -6.41644 LUMO: 0.35919 factor:1 | -1 (0.27791) | -1 | -1 |
| G: -6257.17264 HOMO: -8.88180 LUMO: 1.02315 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.79540 HOMO: -6.41917 LUMO: 1.73064 factor:1 | 1 (-0.25707) | -1 | -1 |
| G: -6257.17264 HOMO: -8.88180 LUMO: 1.02315 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.37977 HOMO: -4.64226 LUMO: -0.87893 factor:1 | -1 (0.15856) | -1 | -1 |
| G: -6257.17264 HOMO: -8.88180 LUMO: 1.02315 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.89148 HOMO: -6.59604 LUMO: 0.90342 factor:1 | 1 (-0.35315) | -1 | -1 |
| G: -6257.17264 HOMO: -8.88180 LUMO: 1.02315 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.89268 HOMO: -6.79468 LUMO: 0.50069 factor:1 | 1 (-0.35435) | -1 | -1 |
| G: -6257.17264 HOMO: -8.88180 LUMO: 1.02315 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.73235 HOMO: -7.04503 LUMO: 0.52518 factor:1 | 1 (-0.19402) | -1 | -1 |
| G: -6257.17264 HOMO: -8.88180 LUMO: 1.02315 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.85232 HOMO: -6.69400 LUMO: 0.54423 factor:1 | 1 (-0.31399) | -1 | -1 |
| G: -6257.17264 HOMO: -8.88180 LUMO: 1.02315 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.83923 HOMO: -6.51713 LUMO: 0.95240 factor:1 | 1 (-0.30090) | -1 | -1 |
| G: -6257.17264 HOMO: -8.88180 LUMO: 1.02315 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.54867 HOMO: -6.88176 LUMO: 1.79323 factor:1 | 1 (-0.01034) | -1 | -1 |
| G: -6257.17264 HOMO: -8.88180 LUMO: 1.02315 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.84936 HOMO: -6.71849 LUMO: 0.28844 factor:1 | 1 (-0.31103) | -1 | -1 |
| G: -6257.17264 HOMO: -8.88180 LUMO: 1.02315 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.63082 HOMO: -6.94979 LUMO: 0.51974 factor:1 | 1 (-0.09249) | -1 | -1 |
| G: -6257.17264 HOMO: -8.88180 LUMO: 1.02315 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.77570 HOMO: -6.76203 LUMO: 0.94151 factor:1 | 1 (-0.23736) | -1 | -1 |
| G: -6257.17264 HOMO: -8.88180 LUMO: 1.02315 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.90125 HOMO: -6.91169 LUMO: 0.89525 factor:1 | 1 (-0.36292) | -1 | -1 |
| G: -6257.17264 HOMO: -8.88180 LUMO: 1.02315 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.91543 HOMO: -6.83006 LUMO: 0.89253 factor:1 | 1 (-0.37710) | -1 | -1 |
| G: -6257.17264 HOMO: -8.88180 LUMO: 1.02315 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.90963 HOMO: -7.08857 LUMO: 0.60409 factor:1 | 1 (-0.37130) | -1 | -1 |
| G: -6257.17264 HOMO: -8.88180 LUMO: 1.02315 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.70187 HOMO: -6.91713 LUMO: 1.76330 factor:1 | 1 (-0.16354) | -1 | -1 |
| G: -6257.17264 HOMO: -8.88180 LUMO: 1.02315 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.78941 HOMO: -6.47359 LUMO: 1.56193 factor:1 | 1 (-0.25108) | -1 | -1 |
| G: -6257.17264 HOMO: -6.91169 LUMO: -0.53879 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.56812 HOMO: -7.00149 LUMO: 1.47214 factor:1 | 1 (-1.02979) | -1 | -1 |
| G: -6257.17264 HOMO: -6.91169 LUMO: -0.53879 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.50893 HOMO: -7.03686 LUMO: 1.97283 factor:1 | 1 (-0.97060) | -1 | -1 |
| G: -6257.17264 HOMO: -6.91169 LUMO: -0.53879 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.55459 HOMO: -7.00965 LUMO: 1.64629 factor:1 | 1 (-1.01626) | -1 | -1 |
| G: -6257.17264 HOMO: -6.91169 LUMO: -0.53879 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.59323 HOMO: -7.06952 LUMO: 1.67622 factor:1 | 1 (-1.05490) | 1 | -1 |
| G: -6257.17264 HOMO: -6.91169 LUMO: -0.53879 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.44588 HOMO: -6.80557 LUMO: 1.70615 factor:1 | 1 (-0.90755) | -1 | -1 |
| G: -6257.17264 HOMO: -6.91169 LUMO: -0.53879 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.45884 HOMO: -6.80829 LUMO: 1.71704 factor:1 | 1 (-0.92051) | -1 | -1 |
| G: -6257.17264 HOMO: -6.91169 LUMO: -0.53879 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.18817 HOMO: -7.26544 LUMO: 1.89935 factor:1 | 1 (-0.64984) | 1 | -1 |
| G: -6257.17264 HOMO: -7.29809 LUMO: 2.83543 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.36762 HOMO: -7.00149 LUMO: 1.47214 factor:1 | 1 (-0.82929) | -1 | -1 |
| G: -6257.17264 HOMO: -7.29809 LUMO: 2.83543 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.61168 HOMO: -7.03686 LUMO: 1.97283 factor:1 | 1 (-1.07335) | -1 | -1 |
| G: -6257.17264 HOMO: -7.29809 LUMO: 2.83543 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.49402 HOMO: -7.00965 LUMO: 1.64629 factor:1 | 1 (-0.95569) | -1 | -1 |
| G: -6257.17264 HOMO: -7.29809 LUMO: 2.83543 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.35258 HOMO: -7.06952 LUMO: 1.67622 factor:1 | 1 (-0.81425) | -1 | -1 |
| G: -6257.17264 HOMO: -7.29809 LUMO: 2.83543 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.32752 HOMO: -6.80557 LUMO: 1.70615 factor:1 | 1 (-0.78918) | -1 | -1 |
| G: -6257.17264 HOMO: -7.29809 LUMO: 2.83543 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.39737 HOMO: -6.80829 LUMO: 1.71704 factor:1 | 1 (-0.85904) | -1 | -1 |
| G: -6257.17264 HOMO: -7.29809 LUMO: 2.83543 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.41280 HOMO: -7.26544 LUMO: 1.89935 factor:1 | 1 (-0.87447) | -1 | -1 |
| G: -6257.17264 HOMO: -7.85865 LUMO: 2.83543 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.12716 HOMO: -7.00149 LUMO: 1.75241 factor:1 | 1 (-0.58883) | -1 | -1 |
| G: -6257.17264 HOMO: -7.85865 LUMO: 2.83543 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.31497 HOMO: -6.91169 LUMO: 2.07079 factor:1 | 1 (-0.77664) | -1 | -1 |
| G: -6257.17264 HOMO: -7.85865 LUMO: 2.83543 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.90392 HOMO: -7.11034 LUMO: 1.76330 factor:1 | 1 (-0.36558) | -1 | -1 |
| G: -6257.17264 HOMO: -7.85865 LUMO: 2.83543 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.67308 HOMO: -6.87360 LUMO: 2.02725 factor:1 | 1 (-0.13475) | -1 | -1 |
| G: -6257.17264 HOMO: -7.85865 LUMO: 2.83543 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.78808 HOMO: -7.08584 LUMO: 1.82044 factor:1 | 1 (-0.24975) | -1 | -1 |
| G: -6257.17264 HOMO: -7.85865 LUMO: 2.83543 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.57552 HOMO: -6.90625 LUMO: 1.68166 factor:1 | 1 (-1.03719) | -1 | -1 |
| G: -6257.17264 HOMO: -7.85865 LUMO: 2.83543 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.68622 HOMO: -6.71577 LUMO: 1.93201 factor:1 | 1 (-1.14789) | -1 | -1 |
| G: -6257.17264 HOMO: -7.85865 LUMO: 2.83543 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.38402 HOMO: -6.99605 LUMO: 2.08439 factor:1 | 1 (-1.84569) | -1 | -1 |
| G: -6257.17264 HOMO: -7.85865 LUMO: 2.83543 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.30242 HOMO: -7.02326 LUMO: 1.97010 factor:1 | 1 (-1.76409) | -1 | -1 |
| G: -6257.17264 HOMO: -7.85865 LUMO: 2.83543 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.69574 HOMO: -6.99877 LUMO: 2.15514 factor:1 | 1 (-1.15741) | -1 | -1 |
| G: -6257.17264 HOMO: -7.85865 LUMO: 2.83543 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.32936 HOMO: -6.75387 LUMO: 1.95106 factor:1 | 1 (-1.79103) | -1 | -1 |
| G: -6257.17264 HOMO: -7.85865 LUMO: 2.83543 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.31957 HOMO: -7.10761 LUMO: 2.06262 factor:1 | 1 (-0.78124) | -1 | -1 |
| G: -6257.17264 HOMO: -7.85865 LUMO: 2.83543 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.81588 HOMO: -7.03142 LUMO: 1.91568 factor:1 | 1 (-1.27755) | -1 | -1 |
| G: -6257.17264 HOMO: -7.85865 LUMO: 2.83543 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.06478 HOMO: -6.98788 LUMO: 1.98371 factor:1 | 1 (-1.52645) | -1 | -1 |
| G: -6257.17264 HOMO: -7.85865 LUMO: 2.83543 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.50357 HOMO: -6.94707 LUMO: 1.68438 factor:1 | 1 (-0.96524) | -1 | -1 |
| G: -6257.17264 HOMO: -7.85865 LUMO: 2.83543 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.73511 HOMO: -6.88176 LUMO: 2.20684 factor:1 | 1 (-2.19678) | -1 | -1 |
| G: -6257.17264 HOMO: -7.85865 LUMO: 2.83543 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.69759 HOMO: -6.73210 LUMO: 2.18780 factor:1 | 1 (-1.15926) | -1 | -1 |
| G: -6257.17264 HOMO: -7.85865 LUMO: 2.83543 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.50123 HOMO: -6.83822 LUMO: 2.06807 factor:1 | 1 (-0.96290) | -1 | -1 |
| G: -6257.17264 HOMO: -7.85865 LUMO: 2.83543 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.63628 HOMO: -6.78924 LUMO: 2.42181 factor:1 | 1 (-1.09795) | -1 | -1 |
| G: -6257.17264 HOMO: -7.85865 LUMO: 2.83543 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.47897 HOMO: -6.94707 LUMO: 1.71704 factor:1 | 1 (-0.94064) | -1 | -1 |
| G: -6257.17264 HOMO: -7.85865 LUMO: 2.83543 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.35878 HOMO: -6.85183 LUMO: 1.78779 factor:1 | 1 (-0.82045) | -1 | -1 |
| G: -6257.17264 HOMO: -7.85865 LUMO: 2.83543 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.65881 HOMO: -6.98788 LUMO: 1.69799 factor:1 | 1 (-1.12048) | -1 | -1 |
| G: -6257.17264 HOMO: -7.85865 LUMO: 2.83543 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.91561 HOMO: -6.79468 LUMO: 2.04358 factor:1 | 1 (-1.37728) | -1 | -1 |
| G: -6257.17264 HOMO: -7.85865 LUMO: 2.83543 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.69462 HOMO: -6.90081 LUMO: 1.97283 factor:1 | 1 (-1.15629) | -1 | -1 |
| G: -6257.17264 HOMO: -7.85865 LUMO: 2.83543 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.78622 HOMO: -6.79468 LUMO: 2.00820 factor:1 | 1 (-1.24789) | -1 | -1 |
| G: -6257.17264 HOMO: -7.85865 LUMO: 2.83543 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.99569 HOMO: -7.06408 LUMO: 2.29936 factor:1 | 1 (-1.45736) | -1 | -1 |
| G: -6257.17264 HOMO: -7.85865 LUMO: 2.83543 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.66808 HOMO: -6.78924 LUMO: 2.13337 factor:1 | 1 (-2.12975) | -1 | -1 |
| G: -6257.17264 HOMO: -7.85865 LUMO: 2.83543 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.46773 HOMO: -6.79468 LUMO: 2.35106 factor:1 | 1 (-1.92940) | -1 | -1 |
| G: -6257.17264 HOMO: -7.85865 LUMO: 2.83543 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.50604 HOMO: -6.82734 LUMO: 2.16603 factor:1 | 1 (-1.96771) | -1 | -1 |
| G: -6257.17264 HOMO: -7.85865 LUMO: 2.83543 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.81286 HOMO: -6.79740 LUMO: 2.36739 factor:1 | 1 (-1.27453) | -1 | -1 |
| G: -6257.17264 HOMO: -7.85865 LUMO: 2.83543 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.92938 HOMO: -7.14027 LUMO: 2.10888 factor:1 | 1 (-1.39105) | -1 | -1 |
| G: -6257.17264 HOMO: -6.61509 LUMO: -0.23674 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.93414 HOMO: -6.96067 LUMO: 1.59731 factor:1 | 1 (-1.39581) | -1 | -1 |
| G: -6257.17264 HOMO: -6.61509 LUMO: -0.23674 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.53280 HOMO: -6.91169 LUMO: 1.37145 factor:1 | 1 (-0.99447) | -1 | -1 |
| G: -6257.17264 HOMO: -6.61509 LUMO: -0.23674 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.39371 HOMO: -6.94707 LUMO: 1.73064 factor:1 | 1 (-1.85538) | -1 | -1 |
| G: -6257.17264 HOMO: -6.61509 LUMO: -0.23674 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.27393 HOMO: -7.02326 LUMO: 1.41227 factor:1 | 1 (-1.73560) | -1 | -1 |
| G: -6257.17264 HOMO: -6.61509 LUMO: -0.23674 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.81885 HOMO: -6.72121 LUMO: 1.43132 factor:1 | 1 (-0.28052) | -1 | -1 |
| G: -6257.17264 HOMO: -6.61509 LUMO: -0.23674 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.80868 HOMO: -6.51168 LUMO: 1.72520 factor:1 | 1 (-0.27035) | -1 | -1 |
| G: -6257.17264 HOMO: -6.61509 LUMO: -0.23674 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.74021 HOMO: -6.98516 LUMO: 1.92929 factor:1 | 1 (-0.20188) | -1 | -1 |
| G: -6257.17264 HOMO: -6.61509 LUMO: -0.23674 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.69852 HOMO: -6.92802 LUMO: 2.07895 factor:1 | 1 (-1.16018) | -1 | -1 |
| G: -6257.17264 HOMO: -6.61509 LUMO: -0.23674 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.50809 HOMO: -7.02326 LUMO: 1.86398 factor:1 | 1 (-0.96976) | -1 | -1 |
| G: -6257.17264 HOMO: -6.61509 LUMO: -0.23674 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.79768 HOMO: -6.82462 LUMO: 1.86670 factor:1 | 1 (-0.25935) | -1 | -1 |
| G: -6257.17264 HOMO: -6.61509 LUMO: -0.23674 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.81499 HOMO: -6.83278 LUMO: 1.71160 factor:1 | 1 (-0.27666) | -1 | -1 |
| G: -6257.17264 HOMO: -6.61509 LUMO: -0.23674 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.59473 HOMO: -6.62869 LUMO: 1.69527 factor:1 | 1 (-1.05640) | -1 | -1 |
| G: -6257.17264 HOMO: -6.61509 LUMO: -0.23674 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.45378 HOMO: -6.84094 LUMO: 1.27349 factor:1 | 1 (-0.91545) | -1 | -1 |
| G: -6257.17264 HOMO: -6.61509 LUMO: -0.23674 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.58011 HOMO: -7.07768 LUMO: 1.27621 factor:1 | 1 (-2.04178) | 1 | -1 |
| G: -6257.17264 HOMO: -6.61509 LUMO: -0.23674 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.79966 HOMO: -7.06135 LUMO: 1.55105 factor:1 | 1 (-1.26133) | 1 | -1 |
| G: -6257.17264 HOMO: -6.61509 LUMO: -0.23674 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.81185 HOMO: -6.94162 LUMO: 1.64629 factor:1 | 1 (-1.27352) | -1 | -1 |
| G: -6257.17264 HOMO: -6.61509 LUMO: -0.23674 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.70999 HOMO: -7.07224 LUMO: 1.65445 factor:1 | 1 (-2.17166) | 1 | -1 |
| G: -6257.17264 HOMO: -6.61509 LUMO: -0.23674 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.97770 HOMO: -6.68584 LUMO: 1.91296 factor:1 | 1 (-2.43936) | -1 | -1 |
| G: -6257.17264 HOMO: -6.61509 LUMO: -0.23674 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.59060 HOMO: -7.09129 LUMO: 1.73609 factor:1 | 1 (-1.05226) | 1 | -1 |
| G: -6257.17264 HOMO: -6.61509 LUMO: -0.23674 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.97187 HOMO: -7.01237 LUMO: 2.01092 factor:1 | 1 (-2.43354) | -1 | -1 |
| G: -6257.17264 HOMO: -6.61509 LUMO: -0.23674 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.61695 HOMO: -6.93618 LUMO: 1.63540 factor:1 | 1 (-2.07862) | -1 | -1 |
| G: -6257.17264 HOMO: -6.61509 LUMO: -0.23674 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.84665 HOMO: -6.98516 LUMO: 1.64629 factor:1 | 1 (-1.30832) | -1 | -1 |
| G: -6257.17264 HOMO: -6.61509 LUMO: -0.23674 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.24233 HOMO: -6.80285 LUMO: 1.95106 factor:1 | 1 (-1.70400) | -1 | -1 |
| G: -6257.17264 HOMO: -6.61509 LUMO: -0.23674 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.28084 HOMO: -6.76747 LUMO: 1.88303 factor:1 | 1 (-1.74251) | -1 | -1 |
| G: -6257.17264 HOMO: -6.61509 LUMO: -0.23674 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.20555 HOMO: -6.64230 LUMO: 1.90480 factor:1 | 1 (-1.66721) | -1 | -1 |
| G: -6257.17264 HOMO: -6.61509 LUMO: -0.23674 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.65236 HOMO: -6.93618 LUMO: 2.19324 factor:1 | 1 (-1.11403) | -1 | -1 |
| G: -6257.17264 HOMO: -6.61509 LUMO: -0.23674 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.22304 HOMO: -6.95523 LUMO: 1.80684 factor:1 | 1 (-1.68471) | -1 | -1 |
| G: -6257.17264 HOMO: -6.61509 LUMO: -0.23674 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.98698 HOMO: -6.66135 LUMO: 1.72792 factor:1 | 1 (-1.44865) | -1 | -1 |
| G: -6257.17264 HOMO: -6.61509 LUMO: -0.23674 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.11711 HOMO: -6.36202 LUMO: 1.89391 factor:1 | 1 (-1.57878) | -1 | -1 |
| G: -6257.17264 HOMO: -6.61509 LUMO: -0.23674 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.16505 HOMO: -7.03959 LUMO: 2.06262 factor:1 | 1 (-1.62672) | -1 | -1 |
| G: -6257.17264 HOMO: -6.61509 LUMO: -0.23674 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.71489 HOMO: -7.08584 LUMO: 2.01092 factor:1 | 1 (-2.17656) | 1 | -1 |
| G: -6257.17264 HOMO: -6.80285 LUMO: -0.55783 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12524.16415 HOMO: -6.96067 LUMO: 1.59731 factor:1 | 1 (-2.62582) | -1 | -1 |
| G: -6257.17264 HOMO: -6.80285 LUMO: -0.55783 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.62066 HOMO: -6.91169 LUMO: 1.37145 factor:1 | 1 (-1.08233) | -1 | -1 |
| G: -6257.17264 HOMO: -6.80285 LUMO: -0.55783 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.17994 HOMO: -6.94707 LUMO: 1.73064 factor:1 | 1 (-1.64161) | -1 | -1 |
| G: -6257.17264 HOMO: -6.80285 LUMO: -0.55783 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.24489 HOMO: -7.02326 LUMO: 1.41227 factor:1 | 1 (-1.70656) | -1 | -1 |
| G: -6257.17264 HOMO: -6.80285 LUMO: -0.55783 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.13295 HOMO: -6.72121 LUMO: 1.43132 factor:1 | 1 (-1.59461) | -1 | -1 |
| G: -6257.17264 HOMO: -6.80285 LUMO: -0.55783 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.24233 HOMO: -6.51168 LUMO: 1.72520 factor:1 | 1 (-1.70400) | -1 | -1 |
| G: -6257.17264 HOMO: -6.80285 LUMO: -0.55783 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12524.11865 HOMO: -6.98516 LUMO: 1.92929 factor:1 | 1 (-2.58032) | -1 | -1 |
| G: -6257.17264 HOMO: -6.80285 LUMO: -0.55783 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.84558 HOMO: -6.92802 LUMO: 2.07895 factor:1 | 1 (-2.30725) | -1 | -1 |
| G: -6257.17264 HOMO: -6.80285 LUMO: -0.55783 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.25357 HOMO: -7.02326 LUMO: 1.86398 factor:1 | 1 (-1.71524) | -1 | -1 |
| G: -6257.17264 HOMO: -6.80285 LUMO: -0.55783 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.25643 HOMO: -6.82462 LUMO: 1.86670 factor:1 | 1 (-1.71810) | -1 | -1 |
| G: -6257.17264 HOMO: -6.80285 LUMO: -0.55783 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.05486 HOMO: -6.83278 LUMO: 1.71160 factor:1 | 1 (-0.51653) | -1 | -1 |
| G: -6257.17264 HOMO: -6.80285 LUMO: -0.55783 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.13817 HOMO: -6.62869 LUMO: 1.69527 factor:1 | 1 (-1.59984) | -1 | -1 |
| G: -6257.17264 HOMO: -6.80285 LUMO: -0.55783 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.03760 HOMO: -6.84094 LUMO: 1.27349 factor:1 | 1 (-1.49927) | -1 | -1 |
| G: -6257.17264 HOMO: -6.80285 LUMO: -0.55783 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12524.48108 HOMO: -7.07768 LUMO: 1.27621 factor:1 | 1 (-2.94275) | 1 | -1 |
| G: -6257.17264 HOMO: -6.80285 LUMO: -0.55783 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.42903 HOMO: -7.06135 LUMO: 1.55105 factor:1 | 1 (-1.89070) | 1 | -1 |
| G: -6257.17264 HOMO: -6.80285 LUMO: -0.55783 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.99322 HOMO: -6.94162 LUMO: 1.64629 factor:1 | 1 (-0.45489) | -1 | -1 |
| G: -6257.17264 HOMO: -6.80285 LUMO: -0.55783 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.10179 HOMO: -7.07224 LUMO: 1.65445 factor:1 | 1 (-1.56346) | 1 | -1 |
| G: -6257.17264 HOMO: -6.80285 LUMO: -0.55783 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.97976 HOMO: -6.68584 LUMO: 1.91296 factor:1 | 1 (-2.44143) | -1 | -1 |
| G: -6257.17264 HOMO: -6.80285 LUMO: -0.55783 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.20321 HOMO: -7.09129 LUMO: 1.73609 factor:1 | 1 (-1.66487) | 1 | -1 |
| G: -6257.17264 HOMO: -6.80285 LUMO: -0.55783 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.07561 HOMO: -7.01237 LUMO: 2.01092 factor:1 | 1 (-1.53728) | -1 | -1 |
| G: -6257.17264 HOMO: -6.80285 LUMO: -0.55783 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12524.09479 HOMO: -6.93618 LUMO: 1.63540 factor:1 | 1 (-2.55646) | -1 | -1 |
| G: -6257.17264 HOMO: -6.80285 LUMO: -0.55783 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.56091 HOMO: -6.98516 LUMO: 1.64629 factor:1 | 1 (-1.02258) | -1 | -1 |
| G: -6257.17264 HOMO: -6.80285 LUMO: -0.55783 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.65808 HOMO: -6.80285 LUMO: 1.95106 factor:1 | 1 (-1.11975) | -1 | -1 |
| G: -6257.17264 HOMO: -6.80285 LUMO: -0.55783 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.38912 HOMO: -6.76747 LUMO: 1.88303 factor:1 | 1 (-0.85079) | -1 | -1 |
| G: -6257.17264 HOMO: -6.80285 LUMO: -0.55783 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.48639 HOMO: -6.64230 LUMO: 1.90480 factor:1 | 1 (-1.94806) | -1 | -1 |
| G: -6257.17264 HOMO: -6.80285 LUMO: -0.55783 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.12356 HOMO: -6.93618 LUMO: 2.19324 factor:1 | 1 (-1.58523) | -1 | -1 |
| G: -6257.17264 HOMO: -6.80285 LUMO: -0.55783 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.41271 HOMO: -6.95523 LUMO: 1.80684 factor:1 | 1 (-0.87438) | -1 | -1 |
| G: -6257.17264 HOMO: -6.80285 LUMO: -0.55783 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.59293 HOMO: -6.66135 LUMO: 1.72792 factor:1 | 1 (-2.05460) | -1 | -1 |
| G: -6257.17264 HOMO: -6.80285 LUMO: -0.55783 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.08286 HOMO: -6.36202 LUMO: 1.89391 factor:1 | 1 (-0.54453) | -1 | -1 |
| G: -6257.17264 HOMO: -6.80285 LUMO: -0.55783 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.51328 HOMO: -7.03959 LUMO: 2.06262 factor:1 | 1 (-1.97495) | -1 | -1 |
| G: -6257.17264 HOMO: -6.80285 LUMO: -0.55783 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.60080 HOMO: -7.08584 LUMO: 2.01092 factor:1 | 1 (-1.06247) | 1 | -1 |
| G: -6257.17264 HOMO: -7.16476 LUMO: 2.86264 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.87530 HOMO: -6.96067 LUMO: 1.59731 factor:1 | 1 (-2.33697) | -1 | -1 |
| G: -6257.17264 HOMO: -7.16476 LUMO: 2.86264 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.39687 HOMO: -6.91169 LUMO: 1.37145 factor:1 | 1 (-1.85854) | -1 | -1 |
| G: -6257.17264 HOMO: -7.16476 LUMO: 2.86264 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.22257 HOMO: -6.94707 LUMO: 1.73064 factor:1 | -1 (0.31576) | -1 | -1 |
| G: -6257.17264 HOMO: -7.16476 LUMO: 2.86264 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.22681 HOMO: -7.02326 LUMO: 1.41227 factor:1 | 1 (-0.68848) | -1 | -1 |
| G: -6257.17264 HOMO: -7.16476 LUMO: 2.86264 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.36899 HOMO: -6.72121 LUMO: 1.43132 factor:1 | 1 (-0.83065) | -1 | -1 |
| G: -6257.17264 HOMO: -7.16476 LUMO: 2.86264 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.14923 HOMO: -6.51168 LUMO: 1.72520 factor:1 | 1 (-0.61090) | -1 | -1 |
| G: -6257.17264 HOMO: -7.16476 LUMO: 2.86264 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.08909 HOMO: -6.98516 LUMO: 1.92929 factor:1 | 1 (-0.55076) | -1 | -1 |
| G: -6257.17264 HOMO: -7.16476 LUMO: 2.86264 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.23448 HOMO: -6.92802 LUMO: 2.07895 factor:1 | 1 (-0.69615) | -1 | -1 |
| G: -6257.17264 HOMO: -7.16476 LUMO: 2.86264 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.62151 HOMO: -7.02326 LUMO: 1.86398 factor:1 | 1 (-1.08318) | -1 | -1 |
| G: -6257.17264 HOMO: -7.16476 LUMO: 2.86264 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.26126 HOMO: -6.82462 LUMO: 1.86670 factor:1 | 1 (-0.72292) | -1 | -1 |
| G: -6257.17264 HOMO: -7.16476 LUMO: 2.86264 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.64109 HOMO: -6.83278 LUMO: 1.71160 factor:1 | 1 (-2.10276) | -1 | -1 |
| G: -6257.17264 HOMO: -7.16476 LUMO: 2.86264 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.09920 HOMO: -6.62869 LUMO: 1.69527 factor:1 | 1 (-1.56087) | -1 | -1 |
| G: -6257.17264 HOMO: -7.16476 LUMO: 2.86264 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.65916 HOMO: -6.84094 LUMO: 1.27349 factor:1 | 1 (-2.12083) | -1 | -1 |
| G: -6257.17264 HOMO: -7.16476 LUMO: 2.86264 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.94339 HOMO: -7.07768 LUMO: 1.27621 factor:1 | 1 (-1.40506) | -1 | -1 |
| G: -6257.17264 HOMO: -7.16476 LUMO: 2.86264 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.15041 HOMO: -7.06135 LUMO: 1.55105 factor:1 | 1 (-1.61208) | -1 | -1 |
| G: -6257.17264 HOMO: -7.16476 LUMO: 2.86264 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.33624 HOMO: -6.94162 LUMO: 1.64629 factor:1 | 1 (-1.79791) | -1 | -1 |
| G: -6257.17264 HOMO: -7.16476 LUMO: 2.86264 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.47502 HOMO: -7.07224 LUMO: 1.65445 factor:1 | 1 (-1.93669) | -1 | -1 |
| G: -6257.17264 HOMO: -7.16476 LUMO: 2.86264 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.56104 HOMO: -6.68584 LUMO: 1.91296 factor:1 | 1 (-1.02271) | -1 | -1 |
| G: -6257.17264 HOMO: -7.16476 LUMO: 2.86264 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.72020 HOMO: -7.09129 LUMO: 1.73609 factor:1 | 1 (-1.18187) | -1 | -1 |
| G: -6257.17264 HOMO: -7.16476 LUMO: 2.86264 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.78156 HOMO: -7.01237 LUMO: 2.01092 factor:1 | 1 (-1.24323) | -1 | -1 |
| G: -6257.17264 HOMO: -7.16476 LUMO: 2.86264 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.57699 HOMO: -6.93618 LUMO: 1.63540 factor:1 | 1 (-1.03866) | -1 | -1 |
| G: -6257.17264 HOMO: -7.16476 LUMO: 2.86264 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.38839 HOMO: -6.98516 LUMO: 1.64629 factor:1 | 1 (-0.85006) | -1 | -1 |
| G: -6257.17264 HOMO: -7.16476 LUMO: 2.86264 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.39329 HOMO: -6.80285 LUMO: 1.95106 factor:1 | 1 (-0.85495) | -1 | -1 |
| G: -6257.17264 HOMO: -7.16476 LUMO: 2.86264 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.82047 HOMO: -6.76747 LUMO: 1.88303 factor:1 | 1 (-2.28214) | -1 | -1 |
| G: -6257.17264 HOMO: -7.16476 LUMO: 2.86264 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.47685 HOMO: -6.64230 LUMO: 1.90480 factor:1 | 1 (-0.93852) | -1 | -1 |
| G: -6257.17264 HOMO: -7.16476 LUMO: 2.86264 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.13841 HOMO: -6.93618 LUMO: 2.19324 factor:1 | 1 (-1.60008) | -1 | -1 |
| G: -6257.17264 HOMO: -7.16476 LUMO: 2.86264 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.79826 HOMO: -6.95523 LUMO: 1.80684 factor:1 | 1 (-2.25993) | -1 | -1 |
| G: -6257.17264 HOMO: -7.16476 LUMO: 2.86264 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.98444 HOMO: -6.66135 LUMO: 1.72792 factor:1 | 1 (-2.44611) | -1 | -1 |
| G: -6257.17264 HOMO: -7.16476 LUMO: 2.86264 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.50607 HOMO: -6.36202 LUMO: 1.89391 factor:1 | 1 (-1.96774) | -1 | -1 |
| G: -6257.17264 HOMO: -7.16476 LUMO: 2.86264 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.02494 HOMO: -7.03959 LUMO: 2.06262 factor:1 | 1 (-1.48661) | -1 | -1 |
| G: -6257.17264 HOMO: -7.16476 LUMO: 2.86264 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.10429 HOMO: -7.08584 LUMO: 2.01092 factor:1 | 1 (-1.56596) | -1 | -1 |
| G: -6257.17264 HOMO: -6.50352 LUMO: 2.10888 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.16081 HOMO: -6.96067 LUMO: 1.59731 factor:1 | 1 (-1.62248) | 1 | 1 |
| G: -6257.17264 HOMO: -6.50352 LUMO: 2.10888 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.27447 HOMO: -6.91169 LUMO: 1.37145 factor:1 | 1 (-1.73614) | -1 | -1 |
| G: -6257.17264 HOMO: -6.50352 LUMO: 2.10888 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.30965 HOMO: -6.94707 LUMO: 1.73064 factor:1 | -1 (0.22868) | 1 | 1 |
| G: -6257.17264 HOMO: -6.50352 LUMO: 2.10888 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.41328 HOMO: -7.02326 LUMO: 1.41227 factor:1 | 1 (-1.87495) | -1 | -1 |
| G: -6257.17264 HOMO: -6.50352 LUMO: 2.10888 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.02000 HOMO: -6.72121 LUMO: 1.43132 factor:1 | 1 (-0.48167) | -1 | -1 |
| G: -6257.17264 HOMO: -6.50352 LUMO: 2.10888 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.52716 HOMO: -6.51168 LUMO: 1.72520 factor:1 | 1 (-1.98883) | 1 | 1 |
| G: -6257.17264 HOMO: -6.50352 LUMO: 2.10888 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.02902 HOMO: -6.98516 LUMO: 1.92929 factor:1 | 1 (-1.49069) | 1 | 1 |
| G: -6257.17264 HOMO: -6.50352 LUMO: 2.10888 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12520.54305 HOMO: -6.92802 LUMO: 2.07895 factor:1 | -1 (0.99528) | 1 | 1 |
| G: -6257.17264 HOMO: -6.50352 LUMO: 2.10888 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12520.91228 HOMO: -7.02326 LUMO: 1.86398 factor:1 | -1 (0.62605) | 1 | 1 |
| G: -6257.17264 HOMO: -6.50352 LUMO: 2.10888 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.68272 HOMO: -6.82462 LUMO: 1.86670 factor:1 | 1 (-2.14439) | 1 | 1 |
| G: -6257.17264 HOMO: -6.50352 LUMO: 2.10888 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.79354 HOMO: -6.83278 LUMO: 1.71160 factor:1 | 1 (-1.25521) | 1 | 1 |
| G: -6257.17264 HOMO: -6.50352 LUMO: 2.10888 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.31045 HOMO: -6.62869 LUMO: 1.69527 factor:1 | 1 (-0.77212) | 1 | 1 |
| G: -6257.17264 HOMO: -6.50352 LUMO: 2.10888 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.36956 HOMO: -6.84094 LUMO: 1.27349 factor:1 | 1 (-0.83123) | -1 | -1 |
| G: -6257.17264 HOMO: -6.50352 LUMO: 2.10888 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.38625 HOMO: -7.07768 LUMO: 1.27621 factor:1 | -1 (0.15208) | -1 | -1 |
| G: -6257.17264 HOMO: -6.50352 LUMO: 2.10888 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.29485 HOMO: -7.06135 LUMO: 1.55105 factor:1 | 1 (-1.75652) | -1 | -1 |
| G: -6257.17264 HOMO: -6.50352 LUMO: 2.10888 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.43872 HOMO: -6.94162 LUMO: 1.64629 factor:1 | 1 (-1.90039) | 1 | 1 |
| G: -6257.17264 HOMO: -6.50352 LUMO: 2.10888 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.56243 HOMO: -7.07224 LUMO: 1.65445 factor:1 | 1 (-1.02410) | 1 | 1 |
| G: -6257.17264 HOMO: -6.50352 LUMO: 2.10888 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.74015 HOMO: -6.68584 LUMO: 1.91296 factor:1 | 1 (-1.20182) | 1 | 1 |
| G: -6257.17264 HOMO: -6.50352 LUMO: 2.10888 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.62464 HOMO: -7.09129 LUMO: 1.73609 factor:1 | 1 (-1.08631) | 1 | 1 |
| G: -6257.17264 HOMO: -6.50352 LUMO: 2.10888 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.26097 HOMO: -7.01237 LUMO: 2.01092 factor:1 | -1 (0.27737) | 1 | 1 |
| G: -6257.17264 HOMO: -6.50352 LUMO: 2.10888 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.48463 HOMO: -6.93618 LUMO: 1.63540 factor:1 | 1 (-0.94630) | 1 | 1 |
| G: -6257.17264 HOMO: -6.50352 LUMO: 2.10888 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.48039 HOMO: -6.98516 LUMO: 1.64629 factor:1 | 1 (-0.94206) | 1 | 1 |
| G: -6257.17264 HOMO: -6.50352 LUMO: 2.10888 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.75873 HOMO: -6.80285 LUMO: 1.95106 factor:1 | 1 (-1.22040) | 1 | 1 |
| G: -6257.17264 HOMO: -6.50352 LUMO: 2.10888 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.23889 HOMO: -6.76747 LUMO: 1.88303 factor:1 | 1 (-0.70056) | 1 | 1 |
| G: -6257.17264 HOMO: -6.50352 LUMO: 2.10888 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.34235 HOMO: -6.64230 LUMO: 1.90480 factor:1 | 1 (-0.80401) | 1 | 1 |
| G: -6257.17264 HOMO: -6.50352 LUMO: 2.10888 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.04569 HOMO: -6.93618 LUMO: 2.19324 factor:1 | 1 (-0.50736) | 1 | 1 |
| G: -6257.17264 HOMO: -6.50352 LUMO: 2.10888 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12520.73374 HOMO: -6.95523 LUMO: 1.80684 factor:1 | -1 (0.80459) | 1 | 1 |
| G: -6257.17264 HOMO: -6.50352 LUMO: 2.10888 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.25737 HOMO: -6.66135 LUMO: 1.72792 factor:1 | -1 (0.28096) | 1 | 1 |
| G: -6257.17264 HOMO: -6.50352 LUMO: 2.10888 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.45082 HOMO: -6.36202 LUMO: 1.89391 factor:1 | -1 (0.08751) | -1 | -1 |
| G: -6257.17264 HOMO: -6.50352 LUMO: 2.10888 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.54029 HOMO: -7.03959 LUMO: 2.06262 factor:1 | 1 (-0.00196) | 1 | 1 |
| G: -6257.17264 HOMO: -6.50352 LUMO: 2.10888 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.82952 HOMO: -7.08584 LUMO: 2.01092 factor:1 | 1 (-0.29119) | 1 | 1 |
| G: -6257.17264 HOMO: -6.59604 LUMO: 2.33746 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.08544 HOMO: -6.96067 LUMO: 1.59731 factor:1 | 1 (-0.54711) | 1 | 1 |
| G: -6257.17264 HOMO: -6.59604 LUMO: 2.33746 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.04616 HOMO: -6.91169 LUMO: 1.37145 factor:1 | -1 (0.49217) | -1 | -1 |
| G: -6257.17264 HOMO: -6.59604 LUMO: 2.33746 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.20540 HOMO: -6.94707 LUMO: 1.73064 factor:1 | -1 (0.33293) | 1 | 1 |
| G: -6257.17264 HOMO: -6.59604 LUMO: 2.33746 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.24671 HOMO: -7.02326 LUMO: 1.41227 factor:1 | -1 (0.29162) | -1 | -1 |
| G: -6257.17264 HOMO: -6.59604 LUMO: 2.33746 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.23742 HOMO: -6.72121 LUMO: 1.43132 factor:1 | 1 (-0.69909) | -1 | -1 |
| G: -6257.17264 HOMO: -6.59604 LUMO: 2.33746 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.56269 HOMO: -6.51168 LUMO: 1.72520 factor:1 | 1 (-2.02436) | -1 | -1 |
| G: -6257.17264 HOMO: -6.59604 LUMO: 2.33746 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.60192 HOMO: -6.98516 LUMO: 1.92929 factor:1 | 1 (-1.06358) | 1 | 1 |
| G: -6257.17264 HOMO: -6.59604 LUMO: 2.33746 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12520.36313 HOMO: -6.92802 LUMO: 2.07895 factor:1 | -1 (1.17521) | 1 | 1 |
| G: -6257.17264 HOMO: -6.59604 LUMO: 2.33746 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.43479 HOMO: -7.02326 LUMO: 1.86398 factor:1 | -1 (0.10354) | 1 | 1 |
| G: -6257.17264 HOMO: -6.59604 LUMO: 2.33746 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.00142 HOMO: -6.82462 LUMO: 1.86670 factor:1 | -1 (0.53691) | 1 | 1 |
| G: -6257.17264 HOMO: -6.59604 LUMO: 2.33746 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.66427 HOMO: -6.83278 LUMO: 1.71160 factor:1 | 1 (-0.12593) | 1 | 1 |
| G: -6257.17264 HOMO: -6.59604 LUMO: 2.33746 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.40231 HOMO: -6.62869 LUMO: 1.69527 factor:1 | 1 (-1.86398) | 1 | 1 |
| G: -6257.17264 HOMO: -6.59604 LUMO: 2.33746 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.47922 HOMO: -6.84094 LUMO: 1.27349 factor:1 | 1 (-0.94089) | -1 | -1 |
| G: -6257.17264 HOMO: -6.59604 LUMO: 2.33746 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.50408 HOMO: -7.07768 LUMO: 1.27621 factor:1 | 1 (-1.96575) | -1 | -1 |
| G: -6257.17264 HOMO: -6.59604 LUMO: 2.33746 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.71642 HOMO: -7.06135 LUMO: 1.55105 factor:1 | 1 (-1.17809) | -1 | -1 |
| G: -6257.17264 HOMO: -6.59604 LUMO: 2.33746 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.66023 HOMO: -6.94162 LUMO: 1.64629 factor:1 | 1 (-1.12190) | 1 | 1 |
| G: -6257.17264 HOMO: -6.59604 LUMO: 2.33746 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.37511 HOMO: -7.07224 LUMO: 1.65445 factor:1 | 1 (-0.83678) | 1 | 1 |
| G: -6257.17264 HOMO: -6.59604 LUMO: 2.33746 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.47870 HOMO: -6.68584 LUMO: 1.91296 factor:1 | 1 (-0.94037) | 1 | 1 |
| G: -6257.17264 HOMO: -6.59604 LUMO: 2.33746 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.43870 HOMO: -7.09129 LUMO: 1.73609 factor:1 | 1 (-0.90037) | 1 | 1 |
| G: -6257.17264 HOMO: -6.59604 LUMO: 2.33746 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.25854 HOMO: -7.01237 LUMO: 2.01092 factor:1 | -1 (0.27979) | 1 | 1 |
| G: -6257.17264 HOMO: -6.59604 LUMO: 2.33746 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.50145 HOMO: -6.93618 LUMO: 1.63540 factor:1 | 1 (-0.96312) | 1 | 1 |
| G: -6257.17264 HOMO: -6.59604 LUMO: 2.33746 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.18235 HOMO: -6.98516 LUMO: 1.64629 factor:1 | -1 (0.35598) | 1 | 1 |
| G: -6257.17264 HOMO: -6.59604 LUMO: 2.33746 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.70423 HOMO: -6.80285 LUMO: 1.95106 factor:1 | 1 (-1.16590) | 1 | 1 |
| G: -6257.17264 HOMO: -6.59604 LUMO: 2.33746 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.20158 HOMO: -6.76747 LUMO: 1.88303 factor:1 | 1 (-0.66325) | 1 | 1 |
| G: -6257.17264 HOMO: -6.59604 LUMO: 2.33746 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.03454 HOMO: -6.64230 LUMO: 1.90480 factor:1 | -1 (0.50379) | 1 | 1 |
| G: -6257.17264 HOMO: -6.59604 LUMO: 2.33746 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.13179 HOMO: -6.93618 LUMO: 2.19324 factor:1 | -1 (0.40654) | 1 | 1 |
| G: -6257.17264 HOMO: -6.59604 LUMO: 2.33746 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.84185 HOMO: -6.95523 LUMO: 1.80684 factor:1 | 1 (-0.30352) | 1 | 1 |
| G: -6257.17264 HOMO: -6.59604 LUMO: 2.33746 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.21133 HOMO: -6.66135 LUMO: 1.72792 factor:1 | -1 (0.32700) | 1 | 1 |
| G: -6257.17264 HOMO: -6.59604 LUMO: 2.33746 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12524.31531 HOMO: -6.36202 LUMO: 1.89391 factor:1 | 1 (-2.77698) | -1 | -1 |
| G: -6257.17264 HOMO: -6.59604 LUMO: 2.33746 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12524.00643 HOMO: -7.03959 LUMO: 2.06262 factor:1 | 1 (-2.46810) | 1 | 1 |
| G: -6257.17264 HOMO: -6.59604 LUMO: 2.33746 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.29757 HOMO: -7.08584 LUMO: 2.01092 factor:1 | 1 (-1.75924) | 1 | 1 |
| G: -6257.17264 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12524.14532 HOMO: -7.06135 LUMO: 0.75376 factor:1 | 1 (-2.60699) | 1 | -1 |
| G: -6257.17264 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.90825 HOMO: -5.10213 LUMO: 0.77825 factor:1 | 1 (-2.36992) | -1 | -1 |
| G: -6257.17264 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.30064 HOMO: -5.84228 LUMO: 0.50341 factor:1 | -1 (0.23769) | -1 | -1 |
| G: -6257.17264 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.08240 HOMO: -5.39874 LUMO: 0.68028 factor:1 | 1 (-0.54406) | -1 | -1 |
| G: -6257.17264 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.17622 HOMO: -5.16744 LUMO: 1.14832 factor:1 | 1 (-0.63789) | -1 | -1 |
| G: -6257.17264 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.03513 HOMO: -5.80963 LUMO: 0.35647 factor:1 | 1 (-0.49680) | -1 | -1 |
| G: -6257.17264 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.85231 HOMO: -5.02322 LUMO: 1.07213 factor:1 | 1 (-2.31397) | -1 | -1 |
| G: -6257.17264 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12524.02009 HOMO: -5.80963 LUMO: 0.56328 factor:1 | 1 (-2.48176) | -1 | -1 |
| G: -6257.17264 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.12236 HOMO: -5.45316 LUMO: 0.78369 factor:1 | 1 (-1.58403) | -1 | -1 |
| G: -6257.17264 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.20231 HOMO: -5.25452 LUMO: 0.82178 factor:1 | 1 (-1.66398) | -1 | -1 |
| G: -6257.17264 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12524.28105 HOMO: -5.21370 LUMO: 1.03947 factor:1 | 1 (-2.74272) | -1 | -1 |
| G: -6257.17264 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.67486 HOMO: -6.04365 LUMO: 0.31837 factor:1 | 1 (-2.13653) | -1 | -1 |
| G: -6257.17264 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.08282 HOMO: -5.86405 LUMO: 0.55511 factor:1 | 1 (-1.54449) | -1 | -1 |
| G: -6257.17264 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.38213 HOMO: -5.64908 LUMO: 0.71022 factor:1 | 1 (-0.84380) | -1 | -1 |
| G: -6257.17264 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12524.17253 HOMO: -5.94297 LUMO: 0.68301 factor:1 | 1 (-2.63420) | -1 | -1 |
| G: -6257.17264 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.40182 HOMO: -6.01916 LUMO: 0.56328 factor:1 | 1 (-1.86349) | -1 | -1 |
| G: -6257.17264 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.92546 HOMO: -6.05181 LUMO: 0.35103 factor:1 | 1 (-1.38713) | -1 | -1 |
| G: -6257.17264 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.15452 HOMO: -6.08447 LUMO: 0.48436 factor:1 | 1 (-1.61619) | -1 | -1 |
| G: -6257.17264 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.32553 HOMO: -5.86950 LUMO: 0.36735 factor:1 | 1 (-0.78720) | -1 | -1 |
| G: -6257.17264 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.53766 HOMO: -5.33615 LUMO: 0.65852 factor:1 | 1 (-1.99933) | -1 | -1 |
| G: -6257.17264 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.18438 HOMO: -5.36064 LUMO: 0.86804 factor:1 | 1 (-0.64605) | -1 | -1 |
| G: -6257.17264 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.16040 HOMO: -5.74160 LUMO: 0.64491 factor:1 | 1 (-1.62207) | -1 | -1 |
| G: -6257.17264 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.40005 HOMO: -5.23003 LUMO: 0.66124 factor:1 | 1 (-1.86172) | -1 | -1 |
| G: -6257.17264 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.55070 HOMO: -5.77698 LUMO: 0.84083 factor:1 | 1 (-1.01237) | -1 | -1 |
| G: -6257.17264 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.77829 HOMO: -5.60555 LUMO: 0.84355 factor:1 | 1 (-2.23996) | -1 | -1 |
| G: -6257.17264 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.93286 HOMO: -7.11578 LUMO: -1.62452 factor:1 | 1 (-1.39453) | -1 | -1 |
| G: -6257.17264 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.30070 HOMO: -7.23279 LUMO: -1.63813 factor:1 | 1 (-1.76237) | -1 | -1 |
| G: -6257.17264 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.31005 HOMO: -6.68312 LUMO: -0.88709 factor:1 | -1 (0.22828) | -1 | -1 |
| G: -6257.17264 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.26711 HOMO: -6.99333 LUMO: -0.88709 factor:1 | -1 (0.27122) | -1 | -1 |
| G: -6257.17264 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.29242 HOMO: -7.40694 LUMO: 0.11973 factor:1 | -1 (0.24591) | 1 | 1 |
| G: -6257.17264 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.20790 HOMO: -6.74026 LUMO: -0.72927 factor:1 | -1 (0.33043) | -1 | -1 |
| G: -6257.17264 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.24287 HOMO: -6.67223 LUMO: -0.70750 factor:1 | -1 (0.29546) | -1 | -1 |
| G: -6257.17264 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.06706 HOMO: -7.06952 LUMO: -1.40139 factor:1 | -1 (0.47127) | -1 | -1 |
| G: -6257.17264 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.65471 HOMO: -7.21374 LUMO: -1.13199 factor:1 | 1 (-1.11637) | -1 | -1 |
| G: -6257.17264 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.70173 HOMO: -6.54706 LUMO: -1.34424 factor:1 | 1 (-1.16340) | -1 | -1 |
| G: -6257.17264 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.56679 HOMO: -7.51851 LUMO: -1.05852 factor:1 | 1 (-1.02845) | -1 | -1 |
| G: -6257.17264 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.42578 HOMO: -7.07224 LUMO: -1.89391 factor:1 | 1 (-0.88744) | -1 | -1 |
| G: -6257.17264 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.15988 HOMO: -6.65863 LUMO: -0.46804 factor:1 | 1 (-1.62155) | -1 | -1 |
| G: -6257.17264 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.09997 HOMO: -7.24367 LUMO: 0.29388 factor:1 | 1 (-1.56163) | 1 | 1 |
| G: -6257.17264 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.48609 HOMO: -7.02326 LUMO: -0.87893 factor:1 | 1 (-1.94776) | -1 | -1 |
| G: -6257.17264 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.53956 HOMO: -6.88176 LUMO: 0.71566 factor:1 | 1 (-2.00123) | -1 | -1 |
| G: -6257.17264 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.06223 HOMO: -6.46543 LUMO: 1.01498 factor:1 | 1 (-0.52390) | -1 | -1 |
| G: -6257.17264 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.13649 HOMO: -6.30760 LUMO: 0.17687 factor:1 | 1 (-0.59816) | -1 | -1 |
| G: -6257.17264 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.33712 HOMO: -6.73210 LUMO: -1.06941 factor:1 | 1 (-0.79879) | -1 | -1 |
| G: -6257.17264 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.24923 HOMO: -6.83550 LUMO: -0.75920 factor:1 | 1 (-0.71090) | -1 | -1 |
| G: -6257.17264 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.28477 HOMO: -6.94707 LUMO: 0.42178 factor:1 | 1 (-0.74644) | -1 | -1 |
| G: -6257.17264 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.41388 HOMO: -6.77019 LUMO: -0.38096 factor:1 | 1 (-0.87555) | -1 | -1 |
| G: -6257.17264 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.46442 HOMO: -7.34163 LUMO: 0.35103 factor:1 | 1 (-0.92609) | 1 | 1 |
| G: -6257.17264 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.13486 HOMO: -6.87632 LUMO: -0.87349 factor:1 | 1 (-0.59653) | -1 | -1 |
| G: -6257.17264 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.40681 HOMO: -7.06952 LUMO: -1.47214 factor:1 | 1 (-0.86848) | -1 | -1 |
| G: -6257.17264 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.14359 HOMO: -6.58788 LUMO: -0.37824 factor:1 | 1 (-0.60526) | -1 | -1 |
| G: -6257.17264 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.46768 HOMO: -6.92802 LUMO: -1.24900 factor:1 | 1 (-0.92935) | -1 | -1 |
| G: -6257.17264 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.03954 HOMO: -7.01237 LUMO: -1.31975 factor:1 | 1 (-0.50121) | -1 | -1 |
| G: -6257.17264 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.25200 HOMO: -6.74842 LUMO: 0.45987 factor:1 | 1 (-0.71367) | -1 | -1 |
| G: -6257.17264 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.46178 HOMO: -6.53890 LUMO: 0.94424 factor:1 | 1 (-0.92345) | -1 | -1 |
| G: -6257.17264 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.23777 HOMO: -6.52257 LUMO: -0.66940 factor:1 | 1 (-0.69944) | -1 | -1 |
| G: -6257.17264 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.49525 HOMO: -6.56883 LUMO: -1.48302 factor:1 | 1 (-0.95692) | -1 | -1 |
| G: -6257.17264 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.34406 HOMO: -7.21646 LUMO: 0.13061 factor:1 | 1 (-0.80573) | 1 | 1 |
| G: -6257.17264 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.18727 HOMO: -6.62597 LUMO: -0.64763 factor:1 | 1 (-0.64894) | -1 | -1 |
| G: -6257.17264 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.28207 HOMO: -7.38789 LUMO: 0.31021 factor:1 | 1 (-0.74374) | 1 | 1 |
| G: -6257.17264 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.24686 HOMO: -6.74570 LUMO: -0.70750 factor:1 | 1 (-0.70853) | -1 | -1 |
| G: -6257.17264 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.47070 HOMO: -6.95251 LUMO: -1.25989 factor:1 | 1 (-0.93237) | -1 | -1 |
| G: -6257.17264 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.79128 HOMO: -7.13483 LUMO: -0.76736 factor:1 | 1 (-1.25295) | -1 | -1 |
| G: -6257.17264 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.90350 HOMO: -6.93618 LUMO: -1.24628 factor:1 | 1 (-1.36517) | -1 | -1 |
| G: -6257.17264 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.99939 HOMO: -7.03686 LUMO: 0.26395 factor:1 | 1 (-1.46106) | -1 | -1 |
| G: -6257.17264 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.81604 HOMO: -6.52257 LUMO: -0.84355 factor:1 | 1 (-1.27771) | -1 | -1 |
| G: -6257.17264 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.87456 HOMO: -6.83278 LUMO: -0.49525 factor:1 | 1 (-2.33623) | -1 | -1 |
| G: -6257.17264 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12524.40500 HOMO: -7.18381 LUMO: -1.64629 factor:1 | 1 (-2.86667) | -1 | -1 |
| G: -6257.17264 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.54521 HOMO: -6.74842 LUMO: -0.81090 factor:1 | 1 (-1.00688) | -1 | -1 |
| G: -6257.17264 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.14380 HOMO: -7.09401 LUMO: -0.92519 factor:1 | 1 (-1.60547) | -1 | -1 |
| G: -6257.17264 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.17959 HOMO: -7.20285 LUMO: -0.81634 factor:1 | 1 (-1.64125) | -1 | -1 |
| G: -6257.17264 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.93278 HOMO: -6.72665 LUMO: 0.77008 factor:1 | 1 (-1.39445) | -1 | -1 |
| G: -6257.17264 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.35383 HOMO: -6.80829 LUMO: 0.86532 factor:1 | 1 (-0.81550) | -1 | -1 |
| G: -6257.17264 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.32243 HOMO: -6.20964 LUMO: 0.99866 factor:1 | 1 (-0.78410) | -1 | -1 |
| G: -6257.17264 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.53280 HOMO: -6.52801 LUMO: 1.07757 factor:1 | 1 (-0.99447) | -1 | -1 |
| G: -6257.17264 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.05756 HOMO: -6.74298 LUMO: -0.67756 factor:1 | -1 (0.48077) | -1 | -1 |
| G: -6257.17264 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.88541 HOMO: -7.43959 LUMO: 0.03265 factor:1 | 1 (-0.34708) | 1 | 1 |
| G: -6257.17264 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.32635 HOMO: -6.46815 LUMO: -0.29933 factor:1 | 1 (-0.78801) | -1 | -1 |
| G: -6257.17264 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.24403 HOMO: -6.70489 LUMO: -0.97145 factor:1 | 1 (-0.70570) | -1 | -1 |
| G: -6257.17264 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.87997 HOMO: -6.30216 LUMO: -1.39322 factor:1 | 1 (-0.34164) | -1 | -1 |
| G: -6257.17264 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.28175 HOMO: -7.01782 LUMO: -1.07485 factor:1 | 1 (-0.74342) | -1 | -1 |
| G: -6257.17264 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.11674 HOMO: -6.93074 LUMO: 0.25851 factor:1 | 1 (-0.57841) | -1 | -1 |
| G: -6257.17264 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.04018 HOMO: -7.07224 LUMO: 0.09524 factor:1 | 1 (-1.50185) | 1 | 1 |
| G: -6257.17264 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.16127 HOMO: -6.62325 LUMO: -0.45443 factor:1 | 1 (-1.62294) | -1 | -1 |
| G: -6257.17264 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.72077 HOMO: -7.09945 LUMO: -1.20274 factor:1 | 1 (-2.18243) | -1 | -1 |
| G: -6257.17264 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.81819 HOMO: -6.56067 LUMO: -1.39322 factor:1 | 1 (-1.27986) | -1 | -1 |
| G: -6257.17264 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.82965 HOMO: -6.75387 LUMO: -0.72654 factor:1 | 1 (-1.29132) | -1 | -1 |
| G: -6257.17264 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.30278 HOMO: -6.28583 LUMO: -2.35651 factor:1 | 1 (-0.76445) | -1 | -1 |
| G: -6257.17264 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.24343 HOMO: -6.55522 LUMO: -1.33608 factor:1 | 1 (-0.70510) | -1 | -1 |
| G: -6257.17264 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.78306 HOMO: -7.19741 LUMO: -0.93607 factor:1 | 1 (-1.24473) | -1 | -1 |
| G: -6257.17264 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.86010 HOMO: -6.39740 LUMO: -1.14832 factor:1 | 1 (-1.32177) | -1 | -1 |
| G: -6257.17264 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.23312 HOMO: -7.11850 LUMO: -0.97417 factor:1 | 1 (-0.69479) | -1 | -1 |
| G: -6257.17264 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.14795 HOMO: -6.57699 LUMO: -1.14016 factor:1 | 1 (-0.60962) | -1 | -1 |
| G: -6257.17264 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.77231 HOMO: -6.57699 LUMO: -1.31975 factor:1 | 1 (-1.23398) | -1 | -1 |
| G: -6257.17264 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.66224 HOMO: -6.69128 LUMO: -0.76736 factor:1 | 1 (-1.12391) | -1 | -1 |
| G: -6257.17264 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.18928 HOMO: -7.25728 LUMO: 0.29660 factor:1 | 1 (-0.65095) | 1 | 1 |
| G: -6257.17264 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.98846 HOMO: -6.37019 LUMO: -0.95240 factor:1 | 1 (-0.45013) | -1 | -1 |
| G: -6257.17264 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.41554 HOMO: -6.48447 LUMO: -0.55511 factor:1 | 1 (-1.87720) | -1 | -1 |
| G: -6257.17264 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12524.12137 HOMO: -6.37291 LUMO: -0.78641 factor:1 | 1 (-2.58304) | -1 | -1 |
| G: -6257.17264 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12524.18145 HOMO: -6.65863 LUMO: -0.69933 factor:1 | 1 (-2.64312) | -1 | -1 |
| G: -6257.17264 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.71144 HOMO: -6.44638 LUMO: -0.16055 factor:1 | 1 (-1.17311) | -1 | -1 |
| G: -6257.17264 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.17608 HOMO: -6.41917 LUMO: -0.20136 factor:1 | 1 (-0.63775) | -1 | -1 |
| G: -6257.17264 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.58991 HOMO: -7.33347 LUMO: 0.12789 factor:1 | 1 (-2.05158) | 1 | 1 |
| G: -6257.17264 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12524.07348 HOMO: -6.70489 LUMO: -0.52518 factor:1 | 1 (-2.53515) | -1 | -1 |
| G: -6257.17264 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.12386 HOMO: -7.25183 LUMO: 0.32109 factor:1 | 1 (-1.58553) | 1 | 1 |
| G: -6257.17264 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.86419 HOMO: -7.29265 LUMO: 0.28028 factor:1 | 1 (-0.32586) | 1 | 1 |
| G: -6257.17264 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.18444 HOMO: -6.57155 LUMO: -0.51702 factor:1 | 1 (-0.64611) | -1 | -1 |
| G: -6257.17264 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.92998 HOMO: -7.08040 LUMO: 0.39729 factor:1 | 1 (-0.39165) | 1 | 1 |
| G: -6257.17264 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.53592 HOMO: -6.24501 LUMO: -0.44627 factor:1 | 1 (-1.99759) | -1 | -1 |
| G: -6257.17264 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.93919 HOMO: -6.73754 LUMO: -0.45443 factor:1 | 1 (-2.40086) | -1 | -1 |
| G: -6257.17264 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.12407 HOMO: -6.24501 LUMO: 0.38096 factor:1 | 1 (-1.58574) | -1 | -1 |
| G: -6257.17264 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.62643 HOMO: -6.86815 LUMO: -0.91974 factor:1 | 1 (-1.08810) | -1 | -1 |
| G: -6257.17264 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.82791 HOMO: -7.40150 LUMO: 0.36191 factor:1 | 1 (-0.28958) | 1 | 1 |
| G: -6257.17264 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.06577 HOMO: -6.44094 LUMO: -0.64219 factor:1 | 1 (-0.52744) | -1 | -1 |
| G: -6257.17264 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.62962 HOMO: -6.69944 LUMO: -0.80001 factor:1 | 1 (-1.09129) | -1 | -1 |
| G: -6257.17264 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.88644 HOMO: -6.61509 LUMO: -0.70750 factor:1 | 1 (-1.34811) | -1 | -1 |
| G: -6257.17264 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.72240 HOMO: -7.52123 LUMO: 0.06803 factor:1 | 1 (-2.18407) | 1 | 1 |
| G: -6257.17264 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.58506 HOMO: -7.34163 LUMO: 0.30477 factor:1 | 1 (-2.04673) | 1 | 1 |
| G: -6257.17264 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.10503 HOMO: -6.68584 LUMO: -0.78641 factor:1 | 1 (-1.56670) | -1 | -1 |
| G: -6257.17264 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.55483 HOMO: -6.53890 LUMO: -0.50885 factor:1 | 1 (-2.01650) | -1 | -1 |
| G: -6257.17264 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.85531 HOMO: -6.75659 LUMO: -0.68845 factor:1 | 1 (-1.31698) | -1 | -1 |
| G: -6257.17264 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.88217 HOMO: -7.08857 LUMO: 0.43266 factor:1 | 1 (-1.34383) | 1 | 1 |
| G: -6257.17264 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.18350 HOMO: -6.28583 LUMO: -0.46804 factor:1 | 1 (-1.64517) | -1 | -1 |
| G: -6257.17264 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.32498 HOMO: -6.50080 LUMO: -0.24762 factor:1 | 1 (-0.78665) | -1 | -1 |
| G: -6257.17264 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.28673 HOMO: -6.45454 LUMO: -0.58504 factor:1 | -1 (0.25160) | -1 | -1 |
| G: -6257.17264 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.52709 HOMO: -7.20558 LUMO: 0.20953 factor:1 | -1 (0.01124) | 1 | 1 |
| G: -6257.17264 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12520.63118 HOMO: -6.35930 LUMO: -0.20681 factor:1 | -1 (0.90715) | -1 | -1 |
| G: -6257.17264 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.89485 HOMO: -6.36202 LUMO: -0.14422 factor:1 | 1 (-0.35652) | -1 | -1 |
| G: -6257.17264 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.78612 HOMO: -6.20692 LUMO: 1.97827 factor:1 | 1 (-0.24779) | -1 | -1 |
| G: -6257.17264 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.24695 HOMO: -6.48719 LUMO: 1.74153 factor:1 | -1 (0.29138) | -1 | -1 |
| G: -6257.17264 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.45307 HOMO: -6.84638 LUMO: 1.88575 factor:1 | 1 (-0.91474) | -1 | -1 |
| G: -6257.17264 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.65634 HOMO: -5.90759 LUMO: 2.00820 factor:1 | 1 (-1.11801) | -1 | -1 |
| G: -6257.17264 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.08278 HOMO: -6.56339 LUMO: 1.99732 factor:1 | 1 (-0.54445) | -1 | -1 |
| G: -6257.17264 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.96465 HOMO: -6.20692 LUMO: 1.75241 factor:1 | 1 (-0.42632) | -1 | -1 |
| G: -6257.17264 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.97159 HOMO: -6.16882 LUMO: 1.94017 factor:1 | 1 (-0.43326) | -1 | -1 |
| G: -6257.17264 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.95023 HOMO: -6.80829 LUMO: 1.78507 factor:1 | 1 (-0.41190) | -1 | -1 |
| G: -6257.17264 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.59009 HOMO: -6.58243 LUMO: 1.78235 factor:1 | 1 (-0.05176) | -1 | -1 |
| G: -6257.17264 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.69554 HOMO: -5.85045 LUMO: 1.82316 factor:1 | 1 (-2.15721) | -1 | -1 |
| G: -6257.17264 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.87419 HOMO: -5.93752 LUMO: 1.56465 factor:1 | 1 (-1.33586) | -1 | -1 |
| G: -6257.17264 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.80918 HOMO: -6.59604 LUMO: -0.53334 factor:1 | 1 (-1.27085) | -1 | -1 |
| G: -6257.17264 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.71264 HOMO: -7.06135 LUMO: 0.29660 factor:1 | 1 (-1.17431) | 1 | 1 |
| G: -6257.17264 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.03058 HOMO: -6.50352 LUMO: 1.61908 factor:1 | 1 (-1.49225) | -1 | -1 |
| G: -6257.17264 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.43988 HOMO: -6.68040 LUMO: -0.60681 factor:1 | -1 (0.09845) | -1 | -1 |
| G: -6257.17264 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.73931 HOMO: -6.93618 LUMO: -1.09662 factor:1 | 1 (-1.20097) | -1 | -1 |
| G: -6257.17264 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.48597 HOMO: -6.72121 LUMO: -1.14016 factor:1 | 1 (-0.94764) | -1 | -1 |
| G: -6257.17264 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.98628 HOMO: -7.12394 LUMO: -1.24900 factor:1 | 1 (-0.44795) | -1 | -1 |
| G: -6257.17264 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.89610 HOMO: -6.71305 LUMO: -0.71566 factor:1 | 1 (-1.35777) | -1 | -1 |
| G: -6257.17264 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.74633 HOMO: -7.09401 LUMO: -0.86532 factor:1 | 1 (-1.20800) | -1 | -1 |
| G: -6257.17264 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.99940 HOMO: -7.08584 LUMO: -0.92519 factor:1 | 1 (-0.46107) | -1 | -1 |
| G: -6257.17264 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.57248 HOMO: -7.05591 LUMO: 0.11973 factor:1 | 1 (-0.03415) | -1 | -1 |
| G: -6257.17264 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.56516 HOMO: -7.14843 LUMO: -1.58370 factor:1 | 1 (-0.02683) | -1 | -1 |
| G: -6257.17264 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.76350 HOMO: -7.36884 LUMO: -1.97010 factor:1 | 1 (-1.22517) | -1 | -1 |
| G: -6257.17264 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.67699 HOMO: -6.81373 LUMO: -1.72248 factor:1 | 1 (-1.13866) | -1 | -1 |
| G: -6257.17264 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.22275 HOMO: -6.87360 LUMO: -1.03947 factor:1 | 1 (-0.68442) | -1 | -1 |
| G: -6257.17264 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.65946 HOMO: -7.02870 LUMO: -0.87349 factor:1 | 1 (-2.12113) | -1 | -1 |
| G: -6257.17264 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12524.04738 HOMO: -7.16476 LUMO: -1.18097 factor:1 | 1 (-2.50905) | -1 | -1 |
| G: -6257.17264 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.16342 HOMO: -7.51851 LUMO: 0.07891 factor:1 | 1 (-1.62509) | 1 | 1 |
| G: -6257.17264 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.90148 HOMO: -7.04231 LUMO: -0.83539 factor:1 | 1 (-2.36315) | -1 | -1 |
| G: -6257.17264 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.00176 HOMO: -6.83278 LUMO: -0.60137 factor:1 | 1 (-1.46343) | -1 | -1 |
| G: -6257.17264 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.17567 HOMO: -6.89809 LUMO: -1.19186 factor:1 | 1 (-1.63734) | -1 | -1 |
| G: -6257.17264 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.91833 HOMO: -7.16476 LUMO: -0.79185 factor:1 | 1 (-1.38000) | -1 | -1 |
| G: -6257.17264 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.42191 HOMO: -6.97156 LUMO: -1.25444 factor:1 | 1 (-0.88358) | -1 | -1 |
| G: -6257.17264 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.70951 HOMO: -6.84366 LUMO: -0.88437 factor:1 | 1 (-1.17118) | -1 | -1 |
| G: -6257.17264 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.46575 HOMO: -6.91986 LUMO: -1.12655 factor:1 | 1 (-0.92742) | -1 | -1 |
| G: -6257.17264 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.39972 HOMO: -6.49536 LUMO: -0.29660 factor:1 | -1 (0.13861) | -1 | -1 |
| G: -6257.17264 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.33942 HOMO: -6.74842 LUMO: 0.42450 factor:1 | -1 (0.19892) | -1 | -1 |
| G: -6257.17264 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.94108 HOMO: -7.34435 LUMO: 0.32109 factor:1 | 1 (-1.40275) | 1 | 1 |
| G: -6257.17264 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.06747 HOMO: -7.16476 LUMO: 0.28572 factor:1 | 1 (-1.52914) | 1 | 1 |
| G: -6257.17264 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.29334 HOMO: -6.74298 LUMO: -0.43538 factor:1 | 1 (-0.75501) | -1 | -1 |
| G: -6257.17264 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.11418 HOMO: -7.19469 LUMO: -1.61091 factor:1 | 1 (-0.57585) | -1 | -1 |
| G: -6257.17264 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.87190 HOMO: -7.35252 LUMO: -1.78235 factor:1 | 1 (-2.33357) | -1 | -1 |
| G: -6257.17264 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12524.25231 HOMO: -7.25456 LUMO: -1.66806 factor:1 | 1 (-2.71398) | -1 | -1 |
| G: -6257.17264 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.74561 HOMO: -7.54844 LUMO: -1.07213 factor:1 | 1 (-2.20728) | -1 | -1 |
| G: -6257.17264 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12524.04194 HOMO: -7.21918 LUMO: -1.55377 factor:1 | 1 (-2.50361) | -1 | -1 |
| G: -6257.17264 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.94232 HOMO: -7.01782 LUMO: -1.60547 factor:1 | 1 (-2.40399) | -1 | -1 |
| G: -6257.17264 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.23186 HOMO: -7.21646 LUMO: -1.53472 factor:1 | 1 (-1.69353) | -1 | -1 |
| G: -6257.17264 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.06327 HOMO: -6.73754 LUMO: -1.37417 factor:1 | 1 (-0.52493) | -1 | -1 |
| G: -6257.17264 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.88548 HOMO: -6.78924 LUMO: 0.66396 factor:1 | 1 (-1.34715) | -1 | -1 |
| G: -6257.17264 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.90157 HOMO: -6.82734 LUMO: 0.61226 factor:1 | 1 (-1.36324) | -1 | -1 |
| G: -6257.17264 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.85052 HOMO: -6.74026 LUMO: 0.65579 factor:1 | 1 (-1.31219) | -1 | -1 |
| G: -6257.17264 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.16980 HOMO: -7.10489 LUMO: -1.30887 factor:1 | 1 (-0.63147) | -1 | -1 |
| G: -6257.17264 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.73492 HOMO: -7.05047 LUMO: 0.42722 factor:1 | 1 (-2.19658) | -1 | -1 |
| G: -6257.17264 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.66286 HOMO: -6.61237 LUMO: 1.30887 factor:1 | 1 (-2.12453) | -1 | -1 |
| G: -6257.17264 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.10824 HOMO: -7.05863 LUMO: 0.59049 factor:1 | 1 (-1.56991) | -1 | -1 |
| G: -6257.17264 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.86836 HOMO: -6.26406 LUMO: 0.78641 factor:1 | 1 (-2.33003) | -1 | -1 |
| G: -6257.17264 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.13763 HOMO: -6.70489 LUMO: 0.67756 factor:1 | 1 (-1.59929) | -1 | -1 |
| G: -6257.17264 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.14179 HOMO: -6.78652 LUMO: -0.94968 factor:1 | 1 (-1.60346) | -1 | -1 |
| G: -6257.17264 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.27560 HOMO: -6.36202 LUMO: -0.94424 factor:1 | -1 (0.26273) | -1 | -1 |
| G: -6257.17264 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.27626 HOMO: -6.81645 LUMO: -1.09934 factor:1 | -1 (0.26207) | -1 | -1 |
| G: -6257.17264 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.95837 HOMO: -7.07224 LUMO: 0.85988 factor:1 | 1 (-0.42003) | 1 | 1 |
| G: -6257.17264 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.04563 HOMO: -7.02326 LUMO: 1.10206 factor:1 | 1 (-0.50730) | -1 | -1 |
| G: -6257.17264 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.92528 HOMO: -6.71305 LUMO: 0.84627 factor:1 | 1 (-0.38695) | -1 | -1 |
| G: -6257.17264 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.04637 HOMO: -7.27360 LUMO: 0.88165 factor:1 | 1 (-0.50804) | 1 | 1 |
| G: -6257.17264 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.12026 HOMO: -6.84911 LUMO: 0.59865 factor:1 | -1 (0.41808) | -1 | -1 |
| G: -6257.17264 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.91057 HOMO: -6.75114 LUMO: -2.49801 factor:1 | 1 (-1.37224) | -1 | -1 |
| G: -6257.17264 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.04592 HOMO: -6.97156 LUMO: 0.53606 factor:1 | 1 (-1.50759) | -1 | -1 |
| G: -6257.17264 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.80289 HOMO: -6.54434 LUMO: 0.73199 factor:1 | 1 (-2.26456) | -1 | -1 |
| G: -6257.17264 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.33151 HOMO: -6.21236 LUMO: 0.99866 factor:1 | 1 (-1.79318) | -1 | -1 |
| G: -6257.17264 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.96486 HOMO: -6.34025 LUMO: 0.50341 factor:1 | 1 (-1.42653) | -1 | -1 |
| G: -6257.17264 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.19051 HOMO: -6.59876 LUMO: -0.69389 factor:1 | -1 (0.34782) | -1 | -1 |
| G: -6257.17264 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.05797 HOMO: -6.54978 LUMO: -1.00682 factor:1 | -1 (0.48036) | -1 | -1 |
| G: -6257.17264 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.88272 HOMO: -6.82462 LUMO: -0.98777 factor:1 | 1 (-0.34439) | -1 | -1 |
| G: -6257.17264 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.83033 HOMO: -6.85455 LUMO: -0.68573 factor:1 | 1 (-1.29200) | -1 | -1 |
| G: -6257.17264 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.59762 HOMO: -7.55388 LUMO: -0.03265 factor:1 | 1 (-1.05928) | 1 | 1 |
| G: -6257.17264 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.14974 HOMO: -6.77019 LUMO: -0.71838 factor:1 | 1 (-0.61141) | -1 | -1 |
| G: -6257.17264 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.91085 HOMO: -6.84911 LUMO: -1.25444 factor:1 | 1 (-1.37252) | -1 | -1 |
| G: -6257.17264 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.86704 HOMO: -6.95251 LUMO: -1.03675 factor:1 | 1 (-0.32871) | -1 | -1 |
| G: -6257.17264 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.00095 HOMO: -6.80829 LUMO: -0.77280 factor:1 | 1 (-0.46262) | -1 | -1 |
| G: -6257.17264 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.83235 HOMO: -6.94162 LUMO: -0.94151 factor:1 | 1 (-0.29402) | -1 | -1 |
| G: -6257.17264 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.68967 HOMO: -6.89809 LUMO: -0.90886 factor:1 | 1 (-1.15134) | -1 | -1 |
| G: -6257.17264 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.95056 HOMO: -6.85183 LUMO: -0.88981 factor:1 | 1 (-0.41223) | -1 | -1 |
| G: -6257.17264 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.69740 HOMO: -6.51985 LUMO: -0.84627 factor:1 | 1 (-1.15907) | -1 | -1 |
| G: -6257.17264 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.97839 HOMO: -6.83278 LUMO: -1.08029 factor:1 | 1 (-0.44006) | -1 | -1 |
| G: -6257.17264 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.94206 HOMO: -6.91986 LUMO: 0.66396 factor:1 | 1 (-1.40373) | -1 | -1 |
| G: -6257.17264 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.72603 HOMO: -6.94162 LUMO: 0.50885 factor:1 | 1 (-1.18770) | -1 | -1 |
| G: -6257.17264 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.84323 HOMO: -6.94435 LUMO: 0.80546 factor:1 | 1 (-1.30489) | -1 | -1 |
| G: -6257.17264 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.93961 HOMO: -6.74298 LUMO: -0.81634 factor:1 | 1 (-1.40128) | -1 | -1 |
| G: -6257.17264 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.02211 HOMO: -7.04503 LUMO: 1.15921 factor:1 | 1 (-1.48378) | -1 | -1 |
| G: -6257.17264 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.07052 HOMO: -6.76475 LUMO: 0.75920 factor:1 | 1 (-1.53219) | -1 | -1 |
| G: -6257.17264 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.15114 HOMO: -7.05047 LUMO: 0.68845 factor:1 | -1 (0.38719) | -1 | -1 |
| G: -6257.17264 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.07850 HOMO: -7.12666 LUMO: 0.60681 factor:1 | 1 (-0.54017) | 1 | 1 |
| G: -6257.17264 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.98552 HOMO: -6.90897 LUMO: -1.22723 factor:1 | 1 (-0.44719) | -1 | -1 |
| G: -6257.17264 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.84100 HOMO: -7.10761 LUMO: 0.58232 factor:1 | 1 (-0.30267) | 1 | 1 |
| G: -6257.17264 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.58737 HOMO: -6.57427 LUMO: 0.71294 factor:1 | 1 (-0.04903) | -1 | -1 |
| G: -6257.17264 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.06767 HOMO: -6.22597 LUMO: 0.99322 factor:1 | 1 (-0.52934) | -1 | -1 |
| G: -6257.17264 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.05739 HOMO: -6.83550 LUMO: -0.77825 factor:1 | 1 (-0.51906) | -1 | -1 |
| G: -6257.17264 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.04582 HOMO: -7.14843 LUMO: 0.44627 factor:1 | 1 (-0.50749) | 1 | 1 |
| G: -6257.17264 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.92707 HOMO: -7.08040 LUMO: 0.78913 factor:1 | 1 (-0.38874) | 1 | 1 |
| G: -6257.17264 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.90917 HOMO: -6.81373 LUMO: -0.93879 factor:1 | 1 (-0.37084) | -1 | -1 |
| G: -6257.17264 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.71572 HOMO: -6.95251 LUMO: 0.22585 factor:1 | 1 (-0.17739) | -1 | -1 |
| G: -6257.17264 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.91744 HOMO: -7.13483 LUMO: -1.25444 factor:1 | 1 (-0.37911) | -1 | -1 |
| G: -6257.17264 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.83841 HOMO: -6.37835 LUMO: -1.54289 factor:1 | 1 (-1.30008) | -1 | -1 |
| G: -6257.17264 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.76769 HOMO: -6.53617 LUMO: -1.43948 factor:1 | 1 (-1.22936) | -1 | -1 |
| G: -6257.17264 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.84233 HOMO: -6.38379 LUMO: 0.16055 factor:1 | 1 (-1.30400) | -1 | -1 |
| G: -6257.17264 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.54853 HOMO: -6.53617 LUMO: 0.15783 factor:1 | 1 (-1.01020) | -1 | -1 |
| G: -6257.17264 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.87030 HOMO: -6.79740 LUMO: -0.17960 factor:1 | 1 (-1.33197) | -1 | -1 |
| G: -6257.17264 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.74722 HOMO: -6.26678 LUMO: -0.41361 factor:1 | 1 (-1.20889) | -1 | -1 |
| G: -6257.17264 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.68635 HOMO: -6.35658 LUMO: -0.24218 factor:1 | 1 (-1.14802) | -1 | -1 |
| G: -6257.17264 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.80924 HOMO: -6.48175 LUMO: -0.71566 factor:1 | 1 (-1.27091) | -1 | -1 |
| G: -6257.17264 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.19154 HOMO: -6.21508 LUMO: -0.40001 factor:1 | 1 (-0.65321) | -1 | -1 |
| G: -6257.17264 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.32379 HOMO: -6.51985 LUMO: -0.32654 factor:1 | 1 (-0.78546) | -1 | -1 |
| G: -6257.17264 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.03741 HOMO: -6.45182 LUMO: -0.66396 factor:1 | 1 (-0.49908) | -1 | -1 |
| G: -6257.17264 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.01880 HOMO: -6.51441 LUMO: -0.65307 factor:1 | 1 (-0.48047) | -1 | -1 |
| G: -6257.17264 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.06411 HOMO: -6.57971 LUMO: -0.92519 factor:1 | 1 (-0.52578) | -1 | -1 |
| G: -6257.17264 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.99815 HOMO: -6.67223 LUMO: -0.58232 factor:1 | 1 (-0.45982) | -1 | -1 |
| G: -6257.17264 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.97001 HOMO: -6.10351 LUMO: -0.45987 factor:1 | 1 (-0.43168) | -1 | -1 |
| G: -6257.17264 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.72480 HOMO: -6.13889 LUMO: -0.50341 factor:1 | 1 (-1.18647) | -1 | -1 |
| G: -6257.17264 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.65484 HOMO: -6.63141 LUMO: -0.28300 factor:1 | 1 (-1.11651) | -1 | -1 |
| G: -6257.17264 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.96954 HOMO: -6.37563 LUMO: -0.22858 factor:1 | 1 (-1.43121) | -1 | -1 |
| G: -6257.17264 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.55555 HOMO: -6.37019 LUMO: 0.11429 factor:1 | 1 (-1.01722) | -1 | -1 |
| G: -6257.17264 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.68989 HOMO: -6.23957 LUMO: 0.28844 factor:1 | 1 (-1.15156) | -1 | -1 |
| G: -6257.17264 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.80943 HOMO: -6.41372 LUMO: -0.53879 factor:1 | 1 (-1.27110) | -1 | -1 |
| G: -6257.17264 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.98316 HOMO: -7.06680 LUMO: 0.32654 factor:1 | 1 (-2.44483) | 1 | 1 |
| G: -6257.17264 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.30895 HOMO: -6.50896 LUMO: -0.73743 factor:1 | 1 (-1.77062) | -1 | -1 |
| G: -6257.17264 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.52269 HOMO: -6.42189 LUMO: -0.28572 factor:1 | 1 (-1.98436) | -1 | -1 |
| G: -6257.17264 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.98814 HOMO: -6.79740 LUMO: -0.25851 factor:1 | 1 (-2.44981) | -1 | -1 |
| G: -6257.17264 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.82132 HOMO: -6.32393 LUMO: 0.17960 factor:1 | 1 (-1.28299) | -1 | -1 |
| G: -6257.17264 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.43718 HOMO: -6.65046 LUMO: 0.03537 factor:1 | 1 (-0.89885) | -1 | -1 |
| G: -6257.17264 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.57933 HOMO: -6.60148 LUMO: 0.07619 factor:1 | 1 (-1.04100) | -1 | -1 |
| G: -6257.17264 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.67517 HOMO: -6.57971 LUMO: 0.11429 factor:1 | 1 (-1.13684) | -1 | -1 |
| G: -6257.17264 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.16823 HOMO: -6.88448 LUMO: -1.21907 factor:1 | -1 (0.37010) | -1 | -1 |
| G: -6257.17264 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.15963 HOMO: -6.97700 LUMO: 0.36463 factor:1 | -1 (0.37870) | -1 | -1 |
| G: -6257.17264 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.74018 HOMO: -6.73210 LUMO: -0.84083 factor:1 | 1 (-1.20185) | -1 | -1 |
| G: -6257.17264 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.66499 HOMO: -6.21236 LUMO: -0.68845 factor:1 | 1 (-1.12666) | -1 | -1 |
| G: -6257.17264 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.88521 HOMO: -6.35658 LUMO: -0.82995 factor:1 | 1 (-1.34688) | -1 | -1 |
| G: -6257.17264 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.38080 HOMO: -6.75114 LUMO: -0.94424 factor:1 | 1 (-0.84246) | -1 | -1 |
| G: -6257.17264 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.33070 HOMO: -6.74026 LUMO: -1.46125 factor:1 | 1 (-0.79237) | -1 | -1 |
| G: -6257.17264 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.35263 HOMO: -7.06952 LUMO: 0.91974 factor:1 | 1 (-0.81430) | 1 | 1 |
| G: -6257.17264 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.78962 HOMO: -7.08857 LUMO: 0.74559 factor:1 | 1 (-1.25129) | 1 | 1 |
| G: -6257.17264 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.18573 HOMO: -6.74298 LUMO: 1.03131 factor:1 | -1 (0.35261) | -1 | -1 |
| G: -6257.17264 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.21196 HOMO: -6.74842 LUMO: -1.77962 factor:1 | -1 (0.32637) | -1 | -1 |
| G: -6257.17264 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.37697 HOMO: -6.82462 LUMO: -1.61908 factor:1 | -1 (0.16136) | -1 | -1 |
| G: -6257.17264 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.11138 HOMO: -7.17020 LUMO: -1.02043 factor:1 | 1 (-0.57304) | -1 | -1 |
| G: -6257.17264 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.76690 HOMO: -6.26406 LUMO: -0.96328 factor:1 | 1 (-1.22857) | -1 | -1 |
| G: -6257.17264 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.30251 HOMO: -6.50896 LUMO: -0.38640 factor:1 | 1 (-0.76418) | -1 | -1 |
| G: -6257.17264 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.30178 HOMO: -7.27632 LUMO: -1.17553 factor:1 | -1 (0.23655) | -1 | -1 |
| G: -6257.17264 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.30872 HOMO: -6.54162 LUMO: -1.36873 factor:1 | -1 (0.22961) | -1 | -1 |
| G: -6257.17264 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.26336 HOMO: -6.42733 LUMO: -1.15648 factor:1 | -1 (0.27497) | -1 | -1 |
| G: -6257.17264 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.11650 HOMO: -6.73754 LUMO: -2.58780 factor:1 | -1 (0.42183) | -1 | -1 |
| G: -6257.17264 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.17032 HOMO: -7.20285 LUMO: 0.75103 factor:1 | -1 (0.36801) | 1 | 1 |
| G: -6257.17264 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.33808 HOMO: -6.98788 LUMO: 0.34831 factor:1 | -1 (0.20025) | -1 | -1 |
| G: -6257.17264 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.88060 HOMO: -6.80013 LUMO: -1.11567 factor:1 | 1 (-0.34226) | -1 | -1 |
| G: -6257.17264 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.86212 HOMO: -6.67767 LUMO: -0.82450 factor:1 | 1 (-0.32379) | -1 | -1 |
| G: -6257.17264 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.79700 HOMO: -6.84911 LUMO: -0.21497 factor:1 | 1 (-0.25867) | -1 | -1 |
| G: -6257.17264 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.37876 HOMO: -6.23141 LUMO: 0.21769 factor:1 | -1 (0.15957) | -1 | -1 |
| G: -6257.17264 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.16809 HOMO: -6.68312 LUMO: 0.16327 factor:1 | -1 (0.37024) | -1 | -1 |
| G: -6257.17264 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.09038 HOMO: -7.04503 LUMO: -1.04220 factor:1 | -1 (0.44795) | -1 | -1 |
| G: -6257.17264 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.00556 HOMO: -6.67495 LUMO: -0.71294 factor:1 | -1 (0.53277) | -1 | -1 |
| G: -6257.17264 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.45647 HOMO: -6.70216 LUMO: -0.55239 factor:1 | 1 (-0.91814) | -1 | -1 |
| G: -6257.17264 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.10231 HOMO: -6.60420 LUMO: -0.71294 factor:1 | 1 (-1.56397) | -1 | -1 |
| G: -6257.17264 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.06923 HOMO: -7.40694 LUMO: 0.11973 factor:1 | -1 (0.46910) | 1 | 1 |
| G: -6257.17264 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12520.89309 HOMO: -6.58788 LUMO: -0.29116 factor:1 | -1 (0.64524) | -1 | -1 |
| G: -6257.17264 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.66028 HOMO: -6.63686 LUMO: -0.32654 factor:1 | 1 (-1.12195) | -1 | -1 |
| G: -6257.17264 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.84772 HOMO: -6.85183 LUMO: -0.95512 factor:1 | 1 (-0.30939) | -1 | -1 |
| G: -6257.17264 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.05937 HOMO: -6.82189 LUMO: -0.88165 factor:1 | 1 (-0.52104) | -1 | -1 |
| G: -6257.17264 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.68519 HOMO: -6.97428 LUMO: -1.03947 factor:1 | 1 (-0.14686) | -1 | -1 |
| G: -6257.17264 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.78027 HOMO: -6.51441 LUMO: -0.05714 factor:1 | 1 (-0.24194) | -1 | -1 |
| G: -6257.17264 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.45406 HOMO: -6.61509 LUMO: -0.77008 factor:1 | -1 (0.08427) | -1 | -1 |
| G: -6257.17264 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.38997 HOMO: -7.36340 LUMO: 0.29116 factor:1 | -1 (0.14836) | 1 | 1 |
| G: -6257.17264 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.49702 HOMO: -6.64230 LUMO: -0.79185 factor:1 | -1 (0.04131) | -1 | -1 |
| G: -6257.17264 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.43969 HOMO: -6.56883 LUMO: -1.03403 factor:1 | -1 (0.09864) | -1 | -1 |
| G: -6257.17264 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.50214 HOMO: -6.69400 LUMO: -0.77825 factor:1 | -1 (0.03619) | -1 | -1 |
| G: -6257.17264 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.59226 HOMO: -6.37019 LUMO: -0.79185 factor:1 | 1 (-0.05393) | -1 | -1 |
| G: -6257.17264 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.53915 HOMO: -6.49808 LUMO: -0.94424 factor:1 | 1 (-0.00082) | -1 | -1 |
| G: -6257.17264 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.53945 HOMO: -6.91713 LUMO: -0.75376 factor:1 | 1 (-0.00112) | -1 | -1 |
| G: -6257.17264 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.63368 HOMO: -7.13755 LUMO: 0.41361 factor:1 | 1 (-0.09535) | 1 | 1 |
| G: -6257.17264 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.62763 HOMO: -7.12122 LUMO: 0.39457 factor:1 | 1 (-1.08930) | 1 | 1 |
| G: -6257.17264 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.70271 HOMO: -6.59332 LUMO: -0.57144 factor:1 | 1 (-1.16438) | -1 | -1 |
| G: -6257.17264 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.73218 HOMO: -6.62325 LUMO: -0.66940 factor:1 | 1 (-1.19385) | -1 | -1 |
| G: -6257.17264 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.54053 HOMO: -6.90897 LUMO: -0.08708 factor:1 | 1 (-1.00220) | -1 | -1 |
| G: -6257.17264 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.14370 HOMO: -6.65591 LUMO: -0.81090 factor:1 | 1 (-0.60537) | -1 | -1 |
| G: -6257.17264 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.22569 HOMO: -6.65318 LUMO: -0.94696 factor:1 | 1 (-0.68736) | -1 | -1 |
| G: -6257.17264 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.12071 HOMO: -6.96067 LUMO: -1.03675 factor:1 | 1 (-0.58238) | -1 | -1 |
| G: -6257.17264 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.20355 HOMO: -6.23141 LUMO: -0.66396 factor:1 | -1 (0.33478) | -1 | -1 |
| G: -6257.17264 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.44379 HOMO: -6.52529 LUMO: -0.78369 factor:1 | 1 (-0.90546) | -1 | -1 |
| G: -6257.17264 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.60115 HOMO: -6.39468 LUMO: -0.40817 factor:1 | 1 (-1.06282) | -1 | -1 |
| G: -6257.17264 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.71193 HOMO: -6.76203 LUMO: -0.20409 factor:1 | 1 (-1.17360) | -1 | -1 |
| G: -6257.17264 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.22368 HOMO: -6.96611 LUMO: -0.90342 factor:1 | 1 (-0.68535) | -1 | -1 |
| G: -6257.17264 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.78448 HOMO: -6.54706 LUMO: -0.87893 factor:1 | 1 (-1.24615) | -1 | -1 |
| G: -6257.17264 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.44453 HOMO: -7.24367 LUMO: -0.97689 factor:1 | -1 (0.09380) | -1 | -1 |
| G: -6257.17264 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.49335 HOMO: -6.61781 LUMO: 1.43404 factor:1 | -1 (0.04498) | -1 | -1 |
| G: -6257.17264 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.39999 HOMO: -6.17971 LUMO: 1.79867 factor:1 | -1 (0.13834) | -1 | -1 |
| G: -6257.17264 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.42894 HOMO: -5.73344 LUMO: 2.13609 factor:1 | -1 (0.10939) | -1 | -1 |
| G: -6257.17264 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.40864 HOMO: -6.72121 LUMO: 2.06807 factor:1 | -1 (0.12969) | -1 | -1 |
| G: -6257.17264 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.19370 HOMO: -6.91169 LUMO: 2.02997 factor:1 | -1 (0.34463) | -1 | -1 |
| G: -6257.17264 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.12243 HOMO: -7.06408 LUMO: 1.41499 factor:1 | -1 (0.41590) | 1 | 1 |
| G: -6257.17264 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.08643 HOMO: -6.94162 LUMO: -0.90070 factor:1 | -1 (0.45190) | -1 | -1 |
| G: -6257.17264 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.96786 HOMO: -7.09401 LUMO: 0.35103 factor:1 | 1 (-0.42953) | 1 | 1 |
| G: -6257.17264 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.06433 HOMO: -6.78652 LUMO: 0.91974 factor:1 | 1 (-0.52600) | -1 | -1 |
| G: -6257.17264 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.54873 HOMO: -6.32937 LUMO: -1.89119 factor:1 | 1 (-0.01039) | -1 | -1 |
| G: -6257.17264 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.75621 HOMO: -7.12666 LUMO: -1.06397 factor:1 | 1 (-0.21788) | -1 | -1 |
| G: -6257.17264 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.00822 HOMO: -6.38107 LUMO: -1.43132 factor:1 | 1 (-0.46989) | -1 | -1 |
| G: -6257.17264 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.02735 HOMO: -7.09129 LUMO: 0.08980 factor:1 | 1 (-0.48902) | 1 | 1 |
| G: -6257.17264 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.00718 HOMO: -6.31304 LUMO: -0.57960 factor:1 | 1 (-0.46885) | -1 | -1 |
| G: -6257.17264 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.00778 HOMO: -6.94435 LUMO: -0.74287 factor:1 | 1 (-0.46945) | -1 | -1 |
| G: -6257.17264 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.05935 HOMO: -6.35658 LUMO: -1.53472 factor:1 | 1 (-0.52102) | -1 | -1 |
| G: -6257.17264 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.49779 HOMO: -6.39740 LUMO: -1.48846 factor:1 | -1 (0.04054) | -1 | -1 |
| G: -6257.17264 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.76473 HOMO: -7.05319 LUMO: -0.33198 factor:1 | 1 (-0.22640) | -1 | -1 |
| G: -6257.17264 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.49057 HOMO: -6.68040 LUMO: -0.09252 factor:1 | -1 (0.04776) | -1 | -1 |
| G: -6257.17264 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.43202 HOMO: -6.35930 LUMO: -0.43266 factor:1 | -1 (0.10631) | -1 | -1 |
| G: -6257.17264 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.43768 HOMO: -6.59604 LUMO: -1.45853 factor:1 | -1 (0.10065) | -1 | -1 |
| G: -6257.17264 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.06463 HOMO: -6.46270 LUMO: -1.49391 factor:1 | -1 (0.47370) | -1 | -1 |
| G: -6257.17264 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12520.81481 HOMO: -7.05863 LUMO: -1.04764 factor:1 | -1 (0.72352) | -1 | -1 |
| G: -6257.17264 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12520.80771 HOMO: -7.14027 LUMO: -0.81634 factor:1 | -1 (0.73063) | -1 | -1 |
| G: -6257.17264 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.96950 HOMO: -6.80285 LUMO: -0.74287 factor:1 | 1 (-0.43116) | -1 | -1 |
| G: -6257.17264 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.08335 HOMO: -6.53890 LUMO: -1.13471 factor:1 | 1 (-0.54502) | -1 | -1 |
| G: -6257.17264 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.17535 HOMO: -6.49808 LUMO: -1.35513 factor:1 | 1 (-0.63702) | -1 | -1 |
| G: -6257.17264 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.33207 HOMO: -6.75931 LUMO: -1.49663 factor:1 | -1 (0.20626) | -1 | -1 |
| G: -6257.17264 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.49011 HOMO: -6.84638 LUMO: -0.77552 factor:1 | -1 (0.04822) | -1 | -1 |
| G: -6257.17264 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.51175 HOMO: -6.65863 LUMO: -1.34696 factor:1 | -1 (0.02659) | -1 | -1 |
| G: -6257.17264 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.99322 HOMO: -6.25590 LUMO: -2.36467 factor:1 | 1 (-0.45489) | -1 | -1 |
| G: -6257.17264 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.28586 HOMO: -7.24911 LUMO: 0.33470 factor:1 | -1 (0.25247) | 1 | 1 |
| G: -6257.17264 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.58554 HOMO: -6.65863 LUMO: -0.75648 factor:1 | 1 (-0.04721) | -1 | -1 |
| G: -6257.17264 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.01799 HOMO: -6.31576 LUMO: -0.83267 factor:1 | 1 (-0.47966) | -1 | -1 |
| G: -6257.17264 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.07127 HOMO: -6.64774 LUMO: -0.66124 factor:1 | 1 (-0.53293) | -1 | -1 |
| G: -6257.17264 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.14563 HOMO: -6.75387 LUMO: -1.00138 factor:1 | 1 (-0.60730) | -1 | -1 |
| G: -6257.17264 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.05556 HOMO: -6.52529 LUMO: -0.68301 factor:1 | 1 (-0.51723) | -1 | -1 |
| G: -6257.17264 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.30395 HOMO: -6.59332 LUMO: -0.68028 factor:1 | 1 (-0.76562) | -1 | -1 |
| G: -6257.17264 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.62168 HOMO: -5.98650 LUMO: 0.31565 factor:1 | 1 (-0.08335) | -1 | -1 |
| G: -6257.17264 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.96003 HOMO: -6.59876 LUMO: 0.22585 factor:1 | 1 (-0.42169) | -1 | -1 |
| G: -6257.17264 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.01061 HOMO: -6.72121 LUMO: 0.10340 factor:1 | 1 (-0.47228) | -1 | -1 |
| G: -6257.17264 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.08098 HOMO: -6.09807 LUMO: 0.20136 factor:1 | 1 (-0.54265) | -1 | -1 |
| G: -6257.17264 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.21965 HOMO: -6.31576 LUMO: 0.06259 factor:1 | 1 (-0.68132) | -1 | -1 |
| G: -6257.17264 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.85698 HOMO: -6.35658 LUMO: -0.58232 factor:1 | 1 (-0.31865) | -1 | -1 |
| G: -6257.17264 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.10721 HOMO: -6.34842 LUMO: -0.55783 factor:1 | 1 (-0.56888) | -1 | -1 |
| G: -6257.17264 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.92321 HOMO: -6.47359 LUMO: -0.57144 factor:1 | 1 (-0.38488) | -1 | -1 |
| G: -6257.17264 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.05524 HOMO: -6.42189 LUMO: -0.09796 factor:1 | 1 (-0.51691) | -1 | -1 |
| G: -6257.17264 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.15789 HOMO: -6.35658 LUMO: -0.31293 factor:1 | -1 (0.38044) | -1 | -1 |
| G: -6257.17264 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12520.94518 HOMO: -7.35524 LUMO: 0.10340 factor:1 | -1 (0.59315) | 1 | 1 |
| G: -6257.17264 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.04824 HOMO: -7.10217 LUMO: 0.36463 factor:1 | 1 (-0.50991) | 1 | 1 |
| G: -6257.17264 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.02740 HOMO: -6.43549 LUMO: -0.56872 factor:1 | 1 (-0.48907) | -1 | -1 |
| G: -6257.17264 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.04672 HOMO: -6.50080 LUMO: -0.71294 factor:1 | 1 (-0.50839) | -1 | -1 |
| G: -6257.17264 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.00337 HOMO: -6.59060 LUMO: -0.57960 factor:1 | 1 (-0.46504) | -1 | -1 |
| G: -6257.17264 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.03094 HOMO: -6.78924 LUMO: -0.31565 factor:1 | 1 (-0.49261) | -1 | -1 |
| G: -6257.17264 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.03967 HOMO: -6.35658 LUMO: 0.07891 factor:1 | 1 (-0.50134) | -1 | -1 |
| G: -6257.17264 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.73039 HOMO: -6.74026 LUMO: -0.87621 factor:1 | 1 (-0.19206) | -1 | -1 |
| G: -6257.17264 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.66603 HOMO: -6.54434 LUMO: 0.81906 factor:1 | 1 (-0.12770) | -1 | -1 |
| G: -6257.17264 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.77752 HOMO: -6.66135 LUMO: 1.40955 factor:1 | 1 (-0.23919) | -1 | -1 |
| G: -6257.17264 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.85831 HOMO: -6.73754 LUMO: -2.54971 factor:1 | 1 (-0.31998) | -1 | -1 |
| G: -6257.17264 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.91202 HOMO: -6.65318 LUMO: 0.69389 factor:1 | 1 (-0.37369) | -1 | -1 |
| G: -6257.17264 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.72941 HOMO: -6.73482 LUMO: 0.62858 factor:1 | 1 (-0.19108) | -1 | -1 |
| G: -6257.17264 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.08182 HOMO: -6.83550 LUMO: 0.68573 factor:1 | 1 (-0.54349) | -1 | -1 |
| G: -6257.17264 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.89028 HOMO: -6.83278 LUMO: 0.45987 factor:1 | 1 (-0.35195) | -1 | -1 |
| G: -6257.17264 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.22928 HOMO: -6.78380 LUMO: 0.68301 factor:1 | 1 (-0.69095) | -1 | -1 |
| G: -6257.17264 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.52930 HOMO: -6.90625 LUMO: 1.36601 factor:1 | -1 (0.00903) | -1 | -1 |
| G: -6257.17264 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.82827 HOMO: -6.82734 LUMO: 1.48302 factor:1 | 1 (-0.28994) | -1 | -1 |
| G: -6257.17264 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.12403 HOMO: -6.44094 LUMO: -0.94424 factor:1 | 1 (-0.58570) | -1 | -1 |
| G: -6257.17264 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.61003 HOMO: -6.91441 LUMO: 0.28844 factor:1 | 1 (-0.07170) | -1 | -1 |
| G: -6257.17264 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.58375 HOMO: -6.49808 LUMO: -0.51157 factor:1 | 1 (-0.04542) | -1 | -1 |
| G: -6257.17264 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.12642 HOMO: -7.09673 LUMO: -0.06259 factor:1 | 1 (-0.58809) | 1 | 1 |
| G: -6257.17264 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.35562 HOMO: -6.77019 LUMO: 0.92247 factor:1 | 1 (-0.81729) | -1 | -1 |
| G: -6257.17264 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.23274 HOMO: -6.75931 LUMO: 1.13744 factor:1 | 1 (-0.69441) | -1 | -1 |
| G: -6257.17264 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.21165 HOMO: -6.15794 LUMO: 1.12383 factor:1 | 1 (-0.67332) | -1 | -1 |
| G: -6257.17264 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.88163 HOMO: -6.59604 LUMO: 1.19458 factor:1 | 1 (-0.34330) | -1 | -1 |
| G: -6257.17264 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.00672 HOMO: -7.09401 LUMO: 0.60137 factor:1 | 1 (-0.46839) | 1 | 1 |
| G: -6257.17264 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.79153 HOMO: -6.34025 LUMO: 0.48164 factor:1 | 1 (-0.25320) | -1 | -1 |
| G: -6257.17264 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.84508 HOMO: -6.72665 LUMO: -2.47624 factor:1 | 1 (-0.30675) | -1 | -1 |
| G: -6257.17264 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.09393 HOMO: -6.48175 LUMO: 0.58232 factor:1 | 1 (-0.55560) | -1 | -1 |
| G: -6257.17264 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.19750 HOMO: -6.94162 LUMO: 0.28300 factor:1 | 1 (-0.65917) | -1 | -1 |
| G: -6257.17264 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.58807 HOMO: -6.65591 LUMO: 0.57144 factor:1 | 1 (-0.04974) | -1 | -1 |
| G: -6257.17264 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.09336 HOMO: -6.58788 LUMO: -1.03947 factor:1 | 1 (-0.55503) | -1 | -1 |
| G: -6257.17264 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.68761 HOMO: -7.18108 LUMO: 0.37824 factor:1 | 1 (-0.14928) | 1 | 1 |
| G: -6257.17264 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.79880 HOMO: -6.63958 LUMO: -1.52112 factor:1 | 1 (-0.26047) | -1 | -1 |
| G: -6257.17264 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.79542 HOMO: -6.12528 LUMO: -0.53606 factor:1 | 1 (-0.25709) | -1 | -1 |
| G: -6257.17264 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.73110 HOMO: -6.22324 LUMO: -0.87893 factor:1 | 1 (-0.19277) | -1 | -1 |
| G: -6257.17264 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.05137 HOMO: -6.62053 LUMO: -0.91974 factor:1 | 1 (-0.51304) | -1 | -1 |
| G: -6257.17264 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.47876 HOMO: -6.84366 LUMO: -0.83811 factor:1 | 1 (-0.94043) | -1 | -1 |
| G: -6257.17264 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.69294 HOMO: -7.26000 LUMO: 0.25851 factor:1 | 1 (-1.15461) | 1 | 1 |
| G: -6257.17264 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.84535 HOMO: -6.49536 LUMO: -0.63403 factor:1 | 1 (-1.30702) | -1 | -1 |
| G: -6257.17264 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.58589 HOMO: -6.45726 LUMO: -0.77825 factor:1 | 1 (-1.04756) | -1 | -1 |
| G: -6257.17264 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.60540 HOMO: -6.74570 LUMO: -0.75103 factor:1 | 1 (-1.06707) | -1 | -1 |
| G: -6257.17264 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.62266 HOMO: -7.20285 LUMO: 0.10612 factor:1 | 1 (-0.08433) | 1 | 1 |
| G: -6257.17264 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.63870 HOMO: -6.45182 LUMO: -0.56600 factor:1 | 1 (-1.10037) | -1 | -1 |
| G: -6257.17264 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.59772 HOMO: -6.83278 LUMO: -0.71838 factor:1 | 1 (-1.05939) | -1 | -1 |
| G: -6257.17264 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.55383 HOMO: -7.01510 LUMO: -1.09662 factor:1 | 1 (-1.01550) | -1 | -1 |
| G: -6257.17264 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.79552 HOMO: -6.48719 LUMO: 0.16871 factor:1 | 1 (-1.25719) | -1 | -1 |
| G: -6257.17264 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.40649 HOMO: -7.30898 LUMO: 0.26667 factor:1 | -1 (0.13184) | 1 | 1 |
| G: -6257.17264 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.47501 HOMO: -6.68856 LUMO: -0.78641 factor:1 | -1 (0.06332) | -1 | -1 |
| G: -6257.17264 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.98737 HOMO: -6.56883 LUMO: -1.00682 factor:1 | 1 (-0.44904) | -1 | -1 |
| G: -6257.17264 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.86498 HOMO: -6.41100 LUMO: -0.48980 factor:1 | 1 (-0.32665) | -1 | -1 |
| G: -6257.17264 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.94389 HOMO: -6.52257 LUMO: -0.59865 factor:1 | 1 (-0.40556) | -1 | -1 |
| G: -6257.17264 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.62715 HOMO: -6.63686 LUMO: -0.56055 factor:1 | 1 (-0.08882) | -1 | -1 |
| G: -6257.17264 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.85216 HOMO: -6.79740 LUMO: -0.75376 factor:1 | 1 (-0.31383) | -1 | -1 |
| G: -6257.17264 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.83869 HOMO: -5.89127 LUMO: 0.22313 factor:1 | 1 (-0.30036) | -1 | -1 |
| G: -6257.17264 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.93611 HOMO: -6.34842 LUMO: 0.11429 factor:1 | 1 (-0.39778) | -1 | -1 |
| G: -6257.17264 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.62160 HOMO: -6.13617 LUMO: 1.94834 factor:1 | 1 (-0.08327) | -1 | -1 |
| G: -6257.17264 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.04512 HOMO: -6.50080 LUMO: 1.74153 factor:1 | 1 (-0.50678) | -1 | -1 |
| G: -6257.17264 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.91153 HOMO: -6.33481 LUMO: 1.68438 factor:1 | 1 (-0.37320) | -1 | -1 |
| G: -6257.17264 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.96087 HOMO: -6.53073 LUMO: 1.95106 factor:1 | 1 (-0.42254) | -1 | -1 |
| G: -6257.17264 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.87172 HOMO: -6.46270 LUMO: 1.89935 factor:1 | 1 (-0.33339) | -1 | -1 |
| G: -6257.17264 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.92000 HOMO: -5.87222 LUMO: 1.91568 factor:1 | 1 (-0.38167) | -1 | -1 |
| G: -6257.17264 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.84560 HOMO: -6.07630 LUMO: 1.81500 factor:1 | 1 (-0.30727) | -1 | -1 |
| G: -6257.17264 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.60364 HOMO: -6.20964 LUMO: 1.81500 factor:1 | 1 (-0.06531) | -1 | -1 |
| G: -6257.17264 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.73325 HOMO: -6.15522 LUMO: 1.90752 factor:1 | 1 (-0.19492) | -1 | -1 |
| G: -6257.17264 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.52173 HOMO: -6.11984 LUMO: 1.95378 factor:1 | -1 (0.01660) | -1 | -1 |
| G: -6257.17264 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.89953 HOMO: -6.58516 LUMO: 2.04358 factor:1 | 1 (-1.36120) | -1 | -1 |
| G: -6257.17264 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.63043 HOMO: -7.37156 LUMO: 0.24490 factor:1 | 1 (-1.09210) | 1 | 1 |
| G: -6257.17264 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.56167 HOMO: -6.36474 LUMO: -0.90070 factor:1 | 1 (-1.02334) | -1 | -1 |
| G: -6257.17264 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.48286 HOMO: -6.43549 LUMO: -0.40817 factor:1 | 1 (-1.94453) | -1 | -1 |
| G: -6257.17264 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12524.17120 HOMO: -7.32258 LUMO: 0.29388 factor:1 | 1 (-2.63286) | 1 | 1 |
| G: -6257.17264 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12524.30905 HOMO: -6.41372 LUMO: -0.20409 factor:1 | 1 (-2.77072) | -1 | -1 |
| G: -6257.17264 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.37243 HOMO: -7.18381 LUMO: 0.42722 factor:1 | 1 (-1.83410) | 1 | 1 |
| G: -6257.17264 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.32321 HOMO: -6.53890 LUMO: -0.54151 factor:1 | 1 (-1.78488) | -1 | -1 |
| G: -6257.17264 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.52593 HOMO: -6.61509 LUMO: 0.08708 factor:1 | 1 (-1.98760) | -1 | -1 |
| G: -6257.17264 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12524.09813 HOMO: -6.78108 LUMO: 2.03541 factor:1 | 1 (-2.55980) | -1 | -1 |
| G: -6257.17264 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.96129 HOMO: -6.50896 LUMO: 1.53472 factor:1 | 1 (-2.42296) | -1 | -1 |
| G: -6257.17264 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12524.13846 HOMO: -6.65591 LUMO: 1.80411 factor:1 | 1 (-2.60013) | -1 | -1 |
| G: -6257.17264 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.45589 HOMO: -6.64502 LUMO: 1.52112 factor:1 | 1 (-1.91756) | -1 | -1 |
| G: -6257.17264 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12524.12113 HOMO: -6.72938 LUMO: 1.48030 factor:1 | 1 (-2.58280) | -1 | -1 |
| G: -6257.17264 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12524.58731 HOMO: -6.16882 LUMO: 1.96466 factor:1 | 1 (-3.04898) | -1 | -1 |
| G: -6257.17264 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.46388 HOMO: -6.22597 LUMO: 1.43132 factor:1 | -1 (0.07445) | -1 | -1 |
| G: -6257.17264 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.45544 HOMO: -6.57699 LUMO: 2.05718 factor:1 | 1 (-0.91711) | -1 | -1 |
| G: -6257.17264 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.22528 HOMO: -6.52529 LUMO: 1.89663 factor:1 | 1 (-0.68695) | -1 | -1 |
| G: -6257.17264 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12524.17193 HOMO: -6.30760 LUMO: 1.88031 factor:1 | 1 (-2.63360) | -1 | -1 |
| G: -6257.17264 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.49543 HOMO: -6.14977 LUMO: 1.92657 factor:1 | 1 (-1.95710) | -1 | -1 |
| G: -6257.17264 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12524.37136 HOMO: -6.20964 LUMO: 1.83949 factor:1 | 1 (-2.83303) | -1 | -1 |
| G: -6257.17264 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.79645 HOMO: -6.31848 LUMO: 1.91296 factor:1 | 1 (-1.25812) | -1 | -1 |
| G: -6257.17264 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.40002 HOMO: -5.80691 LUMO: 2.19868 factor:1 | -1 (0.13832) | -1 | -1 |
| G: -6257.17264 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.52273 HOMO: -6.00827 LUMO: 2.15514 factor:1 | 1 (-0.98440) | -1 | -1 |
| G: -6257.17264 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.50248 HOMO: -6.51713 LUMO: 2.08711 factor:1 | 1 (-0.96415) | -1 | -1 |
| G: -6257.17264 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.40896 HOMO: -6.32937 LUMO: 2.11705 factor:1 | 1 (-0.87063) | -1 | -1 |
| G: -6257.17264 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.53791 HOMO: -6.26678 LUMO: 1.95922 factor:1 | 1 (-0.99958) | -1 | -1 |
| G: -6257.17264 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.92102 HOMO: -6.43005 LUMO: 2.56603 factor:1 | 1 (-1.38269) | -1 | -1 |
| G: -6257.17264 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.50765 HOMO: -6.41644 LUMO: 2.68304 factor:1 | 1 (-0.96932) | -1 | -1 |
| G: -6257.17264 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.31839 HOMO: -5.97834 LUMO: 2.02997 factor:1 | 1 (-1.78006) | -1 | -1 |
| G: -6257.17264 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.31583 HOMO: -6.14161 LUMO: 1.77690 factor:1 | 1 (-1.77750) | -1 | -1 |
| G: -6257.17264 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.52610 HOMO: -6.21508 LUMO: 1.80411 factor:1 | 1 (-1.98776) | -1 | -1 |
| G: -6257.17264 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.28930 HOMO: -6.46270 LUMO: 2.34562 factor:1 | 1 (-1.75097) | -1 | -1 |
| G: -6257.17264 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.65620 HOMO: -6.39195 LUMO: -0.75920 factor:1 | 1 (-1.11787) | -1 | -1 |
| G: -6257.17264 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.99082 HOMO: -7.08584 LUMO: -1.14016 factor:1 | 1 (-1.45249) | -1 | -1 |
| G: -6257.17264 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.12658 HOMO: -6.70216 LUMO: -0.65035 factor:1 | 1 (-1.58825) | -1 | -1 |
| G: -6257.17264 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.99175 HOMO: -6.79468 LUMO: -0.83811 factor:1 | 1 (-1.45341) | -1 | -1 |
| G: -6257.17264 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.44431 HOMO: -6.99877 LUMO: -0.79729 factor:1 | 1 (-0.90598) | -1 | -1 |
| G: -6257.17264 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.58355 HOMO: -7.08040 LUMO: -0.85444 factor:1 | 1 (-1.04522) | -1 | -1 |
| G: -6257.17264 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.67383 HOMO: -7.39333 LUMO: 0.12789 factor:1 | 1 (-1.13550) | 1 | 1 |
| G: -6257.17264 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.56475 HOMO: -7.05047 LUMO: 0.13878 factor:1 | 1 (-0.02642) | -1 | -1 |
| G: -6257.17264 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.26932 HOMO: -6.90897 LUMO: -0.77552 factor:1 | -1 (0.26901) | -1 | -1 |
| G: -6257.17264 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.83972 HOMO: -7.25456 LUMO: 0.05170 factor:1 | 1 (-1.30138) | 1 | 1 |
| G: -6257.17264 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.26192 HOMO: -6.84638 LUMO: -0.84355 factor:1 | -1 (0.27641) | -1 | -1 |
| G: -6257.17264 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.95792 HOMO: -6.78108 LUMO: -0.81634 factor:1 | 1 (-1.41959) | -1 | -1 |
| G: -6257.17264 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.96358 HOMO: -6.74570 LUMO: -0.77280 factor:1 | 1 (-1.42525) | -1 | -1 |
| G: -6257.17264 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.29568 HOMO: -7.28177 LUMO: -1.68438 factor:1 | 1 (-0.75735) | -1 | -1 |
| G: -6257.17264 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.43312 HOMO: -7.22190 LUMO: -1.63540 factor:1 | 1 (-0.89479) | -1 | -1 |
| G: -6257.17264 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.17391 HOMO: -7.15932 LUMO: -1.57554 factor:1 | 1 (-0.63558) | -1 | -1 |
| G: -6257.17264 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.18406 HOMO: -6.57971 LUMO: -0.93063 factor:1 | 1 (-0.64573) | -1 | -1 |
| G: -6257.17264 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.13758 HOMO: -6.88176 LUMO: 0.58232 factor:1 | 1 (-0.59925) | -1 | -1 |
| G: -6257.17264 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.16479 HOMO: -6.85727 LUMO: 0.51430 factor:1 | 1 (-0.62646) | -1 | -1 |
| G: -6257.17264 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12524.13188 HOMO: -6.83550 LUMO: 0.87893 factor:1 | 1 (-2.59354) | -1 | -1 |
| G: -6257.17264 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12524.35163 HOMO: -7.06680 LUMO: 0.87621 factor:1 | 1 (-2.81330) | 1 | 1 |
| G: -6257.17264 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.95448 HOMO: -6.52257 LUMO: 0.81362 factor:1 | 1 (-2.41615) | -1 | -1 |
| G: -6257.17264 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.40231 HOMO: -6.95523 LUMO: 1.17009 factor:1 | 1 (-1.86398) | -1 | -1 |
| G: -6257.17264 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.90943 HOMO: -7.21374 LUMO: 0.97145 factor:1 | 1 (-1.37110) | 1 | 1 |
| G: -6257.17264 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.65658 HOMO: -6.81373 LUMO: -1.54561 factor:1 | 1 (-1.11825) | -1 | -1 |
| G: -6257.17264 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.46491 HOMO: -6.86543 LUMO: -1.52656 factor:1 | -1 (0.07342) | -1 | -1 |
| G: -6257.17264 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.48987 HOMO: -6.90081 LUMO: -0.78097 factor:1 | -1 (0.04846) | -1 | -1 |
| G: -6257.17264 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.50251 HOMO: -6.64502 LUMO: -0.82723 factor:1 | 1 (-0.96418) | -1 | -1 |
| G: -6257.17264 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.45789 HOMO: -6.65591 LUMO: -0.82178 factor:1 | 1 (-0.91955) | -1 | -1 |
| G: -6257.17264 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.37499 HOMO: -6.79468 LUMO: -1.46397 factor:1 | 1 (-1.83666) | -1 | -1 |
| G: -6257.17264 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.93501 HOMO: -7.25728 LUMO: 0.73743 factor:1 | 1 (-1.39668) | 1 | -1 |
| G: -6257.17264 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.98151 HOMO: -7.00149 LUMO: 1.30070 factor:1 | 1 (-1.44318) | -1 | -1 |
| G: -6257.17264 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.03251 HOMO: -7.07768 LUMO: 0.78097 factor:1 | 1 (-1.49418) | 1 | -1 |
| G: -6257.17264 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.88943 HOMO: -6.86271 LUMO: 0.86260 factor:1 | 1 (-1.35110) | -1 | -1 |
| G: -6257.17264 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.93950 HOMO: -6.94707 LUMO: 0.39729 factor:1 | 1 (-1.40117) | -1 | -1 |
| G: -6257.17264 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.35462 HOMO: -6.79740 LUMO: 0.67484 factor:1 | 1 (-0.81629) | -1 | -1 |
| G: -6257.17264 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.36714 HOMO: -6.91986 LUMO: -1.14288 factor:1 | 1 (-0.82880) | -1 | -1 |
| G: -6257.17264 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.87041 HOMO: -6.31576 LUMO: 1.01771 factor:1 | 1 (-1.33208) | -1 | -1 |
| G: -6257.17264 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.96310 HOMO: -6.81645 LUMO: 0.81362 factor:1 | 1 (-0.42477) | -1 | -1 |
| G: -6257.17264 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.79710 HOMO: -6.92258 LUMO: -0.99594 factor:1 | 1 (-1.25877) | -1 | -1 |
| G: -6257.17264 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.36649 HOMO: -6.81373 LUMO: 0.61770 factor:1 | -1 (0.17184) | -1 | -1 |
| G: -6257.17264 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.29909 HOMO: -7.18653 LUMO: 1.19186 factor:1 | -1 (0.23924) | 1 | 1 |
| G: -6257.17264 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.24926 HOMO: -7.00693 LUMO: 0.45715 factor:1 | -1 (0.28907) | -1 | -1 |
| G: -6257.17264 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.11386 HOMO: -7.11306 LUMO: 0.53334 factor:1 | -1 (0.42447) | 1 | 1 |
| G: -6257.17264 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.65636 HOMO: -6.63414 LUMO: -1.64357 factor:1 | 1 (-1.11803) | -1 | -1 |
| G: -6257.17264 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.11158 HOMO: -6.22052 LUMO: -0.74015 factor:1 | 1 (-1.57325) | -1 | -1 |
| G: -6257.17264 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.21375 HOMO: -6.81101 LUMO: -0.50069 factor:1 | -1 (0.32458) | -1 | -1 |
| G: -6257.17264 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.96359 HOMO: -6.71849 LUMO: -0.51974 factor:1 | 1 (-0.42526) | -1 | -1 |
| G: -6257.17264 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.71280 HOMO: -6.72121 LUMO: -1.77690 factor:1 | 1 (-1.17447) | -1 | -1 |
| G: -6257.17264 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.83849 HOMO: -6.94162 LUMO: -1.78779 factor:1 | 1 (-1.30016) | -1 | -1 |
| G: -6257.17264 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.92521 HOMO: -6.91169 LUMO: 0.88981 factor:1 | 1 (-1.38688) | -1 | -1 |
| G: -6257.17264 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.24126 HOMO: -6.97428 LUMO: 0.70750 factor:1 | 1 (-0.70292) | -1 | -1 |
| G: -6257.17264 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.60239 HOMO: -6.74842 LUMO: 1.15921 factor:1 | 1 (-0.06406) | -1 | -1 |
| G: -6257.17264 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.29014 HOMO: -7.25183 LUMO: -0.99594 factor:1 | -1 (0.24820) | -1 | -1 |
| G: -6257.17264 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.68124 HOMO: -6.43821 LUMO: -1.00410 factor:1 | 1 (-0.14291) | -1 | -1 |
| G: -6257.17264 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.44622 HOMO: -6.52257 LUMO: -0.68573 factor:1 | -1 (0.09211) | -1 | -1 |
| G: -6257.17264 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.48192 HOMO: -6.60148 LUMO: -0.52518 factor:1 | -1 (0.05641) | -1 | -1 |
| G: -6257.17264 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.11249 HOMO: -6.07086 LUMO: -1.39594 factor:1 | 1 (-0.57416) | -1 | -1 |
| G: -6257.17264 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.90008 HOMO: -6.78108 LUMO: -1.54833 factor:1 | 1 (-0.36175) | -1 | -1 |
| G: -6257.17264 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.39686 HOMO: -6.73482 LUMO: -1.01498 factor:1 | -1 (0.14147) | -1 | -1 |
| G: -6257.17264 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.99897 HOMO: -6.85183 LUMO: 1.06669 factor:1 | 1 (-0.46063) | -1 | -1 |
| G: -6257.17264 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.98465 HOMO: -6.98516 LUMO: 1.43948 factor:1 | 1 (-0.44632) | -1 | -1 |
| G: -6257.17264 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.89777 HOMO: -6.94162 LUMO: 0.79185 factor:1 | 1 (-0.35944) | -1 | -1 |
| G: -6257.17264 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.95110 HOMO: -6.67495 LUMO: -1.06669 factor:1 | 1 (-0.41277) | -1 | -1 |
| G: -6257.17264 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.98846 HOMO: -6.88720 LUMO: -1.00682 factor:1 | 1 (-0.45013) | -1 | -1 |
| G: -6257.17264 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.95695 HOMO: -6.85999 LUMO: -0.78097 factor:1 | 1 (-0.41862) | -1 | -1 |
| G: -6257.17264 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.72609 HOMO: -6.51713 LUMO: -0.89798 factor:1 | 1 (-0.18776) | -1 | -1 |
| G: -6257.17264 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.83183 HOMO: -6.63141 LUMO: -0.91430 factor:1 | 1 (-0.29350) | -1 | -1 |
| G: -6257.17264 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.33337 HOMO: -6.63414 LUMO: 0.04354 factor:1 | 1 (-0.79504) | -1 | -1 |
| G: -6257.17264 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.19328 HOMO: -6.65046 LUMO: -0.73743 factor:1 | 1 (-0.65495) | -1 | -1 |
| G: -6257.17264 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.40663 HOMO: -6.73754 LUMO: -0.71838 factor:1 | -1 (0.13170) | -1 | -1 |
| G: -6257.17264 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.15860 HOMO: -6.65863 LUMO: -0.60137 factor:1 | -1 (0.37973) | -1 | -1 |
| G: -6257.17264 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.21857 HOMO: -6.61509 LUMO: -0.47892 factor:1 | -1 (0.31976) | -1 | -1 |
| G: -6257.17264 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.20834 HOMO: -6.82189 LUMO: -0.64763 factor:1 | -1 (0.32999) | -1 | -1 |
| G: -6257.17264 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.17754 HOMO: -6.56883 LUMO: -0.51974 factor:1 | -1 (0.36080) | -1 | -1 |
| G: -6257.17264 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.08834 HOMO: -6.97428 LUMO: -0.95512 factor:1 | -1 (0.44999) | -1 | -1 |
| G: -6257.17264 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.32369 HOMO: -6.70489 LUMO: -0.04082 factor:1 | -1 (0.21464) | -1 | -1 |
| G: -6257.17264 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.16401 HOMO: -6.74026 LUMO: 0.02177 factor:1 | -1 (0.37432) | -1 | -1 |
| G: -6257.17264 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.89379 HOMO: -6.50080 LUMO: -0.89525 factor:1 | 1 (-0.35546) | -1 | -1 |
| G: -6257.17264 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.99709 HOMO: -6.46815 LUMO: -0.61226 factor:1 | 1 (-0.45876) | -1 | -1 |
| G: -6257.17264 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.85186 HOMO: -6.57971 LUMO: -0.64219 factor:1 | 1 (-0.31353) | -1 | -1 |
| G: -6257.17264 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.95094 HOMO: -7.17836 LUMO: 0.37280 factor:1 | 1 (-0.41261) | 1 | 1 |
| G: -6257.17264 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12520.83870 HOMO: -6.67223 LUMO: 0.12245 factor:1 | -1 (0.69963) | -1 | -1 |
| G: -6257.17264 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12520.83818 HOMO: -6.55250 LUMO: 0.22858 factor:1 | -1 (0.70015) | -1 | -1 |
| G: -6257.17264 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.22006 HOMO: -6.97156 LUMO: -1.12927 factor:1 | 1 (-0.68173) | -1 | -1 |
| G: -6257.17264 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.10108 HOMO: -6.78924 LUMO: -0.84900 factor:1 | 1 (-1.56275) | -1 | -1 |
| G: -6257.17264 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.21779 HOMO: -6.65046 LUMO: -0.65307 factor:1 | 1 (-1.67946) | -1 | -1 |
| G: -6257.17264 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12520.84180 HOMO: -7.41782 LUMO: 0.08980 factor:1 | -1 (0.69653) | 1 | 1 |
| G: -6257.17264 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.77397 HOMO: -6.56339 LUMO: -0.68573 factor:1 | 1 (-1.23564) | -1 | -1 |
| G: -6257.17264 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.91170 HOMO: -6.31032 LUMO: -0.31837 factor:1 | 1 (-0.37337) | -1 | -1 |
| G: -6257.17264 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.62646 HOMO: -6.72938 LUMO: -0.45987 factor:1 | 1 (-1.08813) | -1 | -1 |
| G: -6257.17264 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.83118 HOMO: -6.59876 LUMO: -1.03131 factor:1 | 1 (-0.29285) | -1 | -1 |
| G: -6257.17264 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.87894 HOMO: -7.29265 LUMO: 0.29660 factor:1 | 1 (-0.34060) | 1 | 1 |
| G: -6257.17264 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.64260 HOMO: -6.42189 LUMO: -0.51157 factor:1 | 1 (-0.10427) | -1 | -1 |
| G: -6257.17264 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.53651 HOMO: -6.27767 LUMO: -0.52790 factor:1 | -1 (0.00182) | -1 | -1 |
| G: -6257.17264 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.48418 HOMO: -6.41644 LUMO: -0.44627 factor:1 | -1 (0.05415) | -1 | -1 |
| G: -6257.17264 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.57117 HOMO: -6.23413 LUMO: -0.52790 factor:1 | 1 (-0.03284) | -1 | -1 |
| G: -6257.17264 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.17500 HOMO: -6.63414 LUMO: -0.44082 factor:1 | 1 (-0.63666) | -1 | -1 |
| G: -6257.17264 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.24885 HOMO: -7.03142 LUMO: 0.47076 factor:1 | 1 (-0.71052) | -1 | -1 |
| G: -6257.17264 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.57353 HOMO: -6.62053 LUMO: -0.14422 factor:1 | 1 (-1.03520) | -1 | -1 |
| G: -6257.17264 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.25187 HOMO: -6.22324 LUMO: 1.96194 factor:1 | 1 (-0.71354) | -1 | -1 |
| G: -6257.17264 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.74263 HOMO: -6.17971 LUMO: 1.71704 factor:1 | 1 (-0.20430) | -1 | -1 |
| G: -6257.17264 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.59893 HOMO: -6.70761 LUMO: 1.68711 factor:1 | 1 (-0.06060) | -1 | -1 |
| G: -6257.17264 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.59275 HOMO: -6.52801 LUMO: 1.56193 factor:1 | 1 (-0.05442) | -1 | -1 |
| G: -6257.17264 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.90056 HOMO: -6.55794 LUMO: 1.52384 factor:1 | 1 (-1.36223) | -1 | -1 |
| G: -6257.17264 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.85259 HOMO: -6.47359 LUMO: 1.82316 factor:1 | 1 (-1.31426) | -1 | -1 |
| G: -6257.17264 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.50121 HOMO: -6.65863 LUMO: 1.83133 factor:1 | 1 (-0.96287) | -1 | -1 |
| G: -6257.17264 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.20487 HOMO: -6.46270 LUMO: 1.90208 factor:1 | 1 (-0.66654) | -1 | -1 |
| G: -6257.17264 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.09989 HOMO: -6.41917 LUMO: 2.03269 factor:1 | 1 (-0.56156) | -1 | -1 |
| G: -6257.17264 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.18321 HOMO: -6.48992 LUMO: 1.87486 factor:1 | 1 (-0.64488) | -1 | -1 |
| G: -6257.17264 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.12264 HOMO: -6.51985 LUMO: 1.69527 factor:1 | 1 (-0.58431) | -1 | -1 |
| G: -6257.17264 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.46306 HOMO: -6.36202 LUMO: 2.05718 factor:1 | -1 (0.07527) | -1 | -1 |
| G: -6257.17264 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.21772 HOMO: -5.96474 LUMO: 1.88575 factor:1 | 1 (-0.67939) | -1 | -1 |
| G: -6257.17264 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.44508 HOMO: -6.56339 LUMO: 2.04630 factor:1 | -1 (0.09325) | -1 | -1 |
| G: -6257.17264 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.66658 HOMO: -6.43277 LUMO: 1.98371 factor:1 | 1 (-0.12825) | -1 | -1 |
| G: -6257.17264 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.34899 HOMO: -6.53345 LUMO: 2.06262 factor:1 | -1 (0.18934) | -1 | -1 |
| G: -6257.17264 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.51131 HOMO: -5.81779 LUMO: 2.11432 factor:1 | -1 (0.02702) | -1 | -1 |
| G: -6257.17264 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.50960 HOMO: -5.91848 LUMO: 1.86942 factor:1 | -1 (0.02874) | -1 | -1 |
| G: -6257.17264 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.29759 HOMO: -6.48447 LUMO: 1.70343 factor:1 | -1 (0.24074) | -1 | -1 |
| G: -6257.17264 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.31865 HOMO: -6.29671 LUMO: -0.89525 factor:1 | -1 (0.21968) | -1 | -1 |
| G: -6257.17264 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.58481 HOMO: -6.63414 LUMO: -0.76192 factor:1 | 1 (-0.04648) | -1 | -1 |
| G: -6257.17264 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.00476 HOMO: -6.56883 LUMO: -0.86260 factor:1 | 1 (-0.46643) | -1 | -1 |
| G: -6257.17264 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.14425 HOMO: -6.93074 LUMO: -0.27483 factor:1 | 1 (-0.60592) | -1 | -1 |
| G: -6257.17264 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.04049 HOMO: -6.85999 LUMO: -0.01905 factor:1 | 1 (-0.50216) | -1 | -1 |
| G: -6257.17264 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.48168 HOMO: -6.26406 LUMO: 0.21769 factor:1 | -1 (0.05665) | -1 | -1 |
| G: -6257.17264 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.60941 HOMO: -6.62325 LUMO: 0.31293 factor:1 | 1 (-0.07108) | -1 | -1 |
| G: -6257.17264 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.64856 HOMO: -6.59604 LUMO: 0.19592 factor:1 | 1 (-1.11022) | -1 | -1 |
| G: -6257.17264 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.65577 HOMO: -6.43277 LUMO: -0.27756 factor:1 | 1 (-1.11744) | -1 | -1 |
| G: -6257.17264 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.41448 HOMO: -6.54978 LUMO: -0.46531 factor:1 | 1 (-0.87615) | -1 | -1 |
| G: -6257.17264 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.97910 HOMO: -6.65046 LUMO: -0.15783 factor:1 | 1 (-0.44077) | -1 | -1 |
| G: -6257.17264 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.59928 HOMO: -7.28721 LUMO: 0.23946 factor:1 | 1 (-0.06095) | 1 | 1 |
| G: -6257.17264 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.75019 HOMO: -6.71849 LUMO: -0.56600 factor:1 | 1 (-1.21186) | -1 | -1 |
| G: -6257.17264 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.72516 HOMO: -6.85183 LUMO: -0.84355 factor:1 | 1 (-1.18682) | -1 | -1 |
| G: -6257.17264 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.69296 HOMO: -6.53345 LUMO: -0.84627 factor:1 | 1 (-1.15463) | -1 | -1 |
| G: -6257.17264 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.53726 HOMO: -6.60148 LUMO: -0.63130 factor:1 | 1 (-0.99893) | -1 | -1 |
| G: -6257.17264 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.84064 HOMO: -6.36202 LUMO: -0.60137 factor:1 | 1 (-1.30231) | -1 | -1 |
| G: -6257.17264 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.65900 HOMO: -6.28855 LUMO: -0.52790 factor:1 | 1 (-1.12067) | -1 | -1 |
| G: -6257.17264 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.80399 HOMO: -7.07224 LUMO: 0.41906 factor:1 | 1 (-1.26566) | 1 | 1 |
| G: -6257.17264 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.59370 HOMO: -6.36202 LUMO: -0.24218 factor:1 | 1 (-1.05537) | -1 | -1 |
| G: -6257.17264 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.96656 HOMO: -6.43549 LUMO: 0.14150 factor:1 | 1 (-0.42823) | -1 | -1 |
| G: -6257.17264 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.13181 HOMO: -6.76747 LUMO: -0.40545 factor:1 | 1 (-0.59348) | -1 | -1 |
| G: -6257.17264 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.28335 HOMO: -6.15249 LUMO: -0.51157 factor:1 | 1 (-0.74502) | -1 | -1 |
| G: -6257.17264 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.14686 HOMO: -6.33753 LUMO: -0.02993 factor:1 | 1 (-0.60853) | -1 | -1 |
| G: -6257.17264 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.45818 HOMO: -6.49808 LUMO: -0.83811 factor:1 | 1 (-0.91985) | -1 | -1 |
| G: -6257.17264 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.12920 HOMO: -6.64502 LUMO: -0.46259 factor:1 | 1 (-0.59087) | -1 | -1 |
| G: -6257.17264 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.93759 HOMO: -6.34570 LUMO: 0.22041 factor:1 | 1 (-1.39926) | -1 | -1 |
| G: -6257.17264 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.84323 HOMO: -6.63414 LUMO: -0.13606 factor:1 | 1 (-1.30489) | -1 | -1 |
| G: -6257.17264 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.84344 HOMO: -6.59604 LUMO: -0.79729 factor:1 | 1 (-1.30511) | -1 | -1 |
| G: -6257.17264 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.72733 HOMO: -7.09401 LUMO: 0.31837 factor:1 | 1 (-1.18900) | 1 | 1 |
| G: -6257.17264 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.71226 HOMO: -6.48719 LUMO: -0.31021 factor:1 | 1 (-1.17393) | -1 | -1 |
| G: -6257.17264 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.48923 HOMO: -7.11306 LUMO: 0.39729 factor:1 | 1 (-0.95090) | 1 | 1 |
| G: -6257.17264 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.66213 HOMO: -6.95251 LUMO: 0.41089 factor:1 | 1 (-1.12380) | -1 | -1 |
| G: -6257.17264 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.39693 HOMO: -6.61509 LUMO: -0.41906 factor:1 | 1 (-0.85860) | -1 | -1 |
| G: -6257.17264 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.48186 HOMO: -6.25318 LUMO: -0.47348 factor:1 | 1 (-0.94353) | -1 | -1 |
| G: -6257.17264 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.65272 HOMO: -6.77019 LUMO: -0.10340 factor:1 | 1 (-1.11439) | -1 | -1 |
| G: -6257.17264 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.65824 HOMO: -6.54706 LUMO: -0.46259 factor:1 | 1 (-1.11991) | -1 | -1 |
| G: -6257.17264 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.58798 HOMO: -6.34297 LUMO: -0.50341 factor:1 | 1 (-1.04965) | -1 | -1 |
| G: -6257.17264 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.77601 HOMO: -6.20692 LUMO: -0.51974 factor:1 | 1 (-1.23768) | -1 | -1 |
| G: -6257.17264 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.73014 HOMO: -7.03686 LUMO: 0.46804 factor:1 | 1 (-1.19180) | -1 | -1 |
| G: -6257.17264 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.33897 HOMO: -6.47087 LUMO: 0.22585 factor:1 | 1 (-0.80064) | -1 | -1 |
| G: -6257.17264 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.08716 HOMO: -6.41917 LUMO: 0.19320 factor:1 | 1 (-0.54883) | -1 | -1 |
| G: -6257.17264 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.28224 HOMO: -6.61237 LUMO: -0.04354 factor:1 | 1 (-0.74390) | -1 | -1 |
| G: -6257.17264 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.30694 HOMO: -6.56339 LUMO: 0.36735 factor:1 | 1 (-0.76861) | -1 | -1 |
| G: -6257.17264 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.21391 HOMO: -6.54978 LUMO: 1.12655 factor:1 | 1 (-0.67558) | -1 | -1 |
| G: -6257.17264 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.16177 HOMO: -6.43277 LUMO: 1.17553 factor:1 | 1 (-0.62344) | -1 | -1 |
| G: -6257.17264 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.17600 HOMO: -6.29944 LUMO: 1.40955 factor:1 | 1 (-0.63767) | -1 | -1 |
| G: -6257.17264 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.18885 HOMO: -6.74842 LUMO: 0.74015 factor:1 | 1 (-0.65052) | -1 | -1 |
| G: -6257.17264 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.89114 HOMO: -6.15522 LUMO: 1.94289 factor:1 | 1 (-1.35281) | -1 | -1 |
| G: -6257.17264 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.86004 HOMO: -6.20147 LUMO: 1.40139 factor:1 | 1 (-1.32171) | -1 | -1 |
| G: -6257.17264 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.07295 HOMO: -6.41100 LUMO: 1.40139 factor:1 | 1 (-0.53462) | -1 | -1 |
| G: -6257.17264 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.15358 HOMO: -6.74570 LUMO: 1.80956 factor:1 | 1 (-0.61525) | -1 | -1 |
| G: -6257.17264 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.65412 HOMO: -6.60148 LUMO: -1.04764 factor:1 | 1 (-0.11578) | -1 | -1 |
| G: -6257.17264 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.10887 HOMO: -6.82734 LUMO: -0.83267 factor:1 | 1 (-0.57054) | -1 | -1 |
| G: -6257.17264 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.75476 HOMO: -7.01782 LUMO: -0.32382 factor:1 | 1 (-1.21643) | -1 | -1 |
| G: -6257.17264 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.28955 HOMO: -6.54434 LUMO: 0.11157 factor:1 | 1 (-1.75122) | -1 | -1 |
| G: -6257.17264 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.77078 HOMO: -6.53617 LUMO: 0.32926 factor:1 | 1 (-2.23245) | -1 | -1 |
| G: -6257.17264 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.77043 HOMO: -6.62597 LUMO: -0.60137 factor:1 | 1 (-2.23210) | -1 | -1 |
| G: -6257.17264 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.87111 HOMO: -6.60965 LUMO: -0.75376 factor:1 | 1 (-2.33278) | -1 | -1 |
| G: -6257.17264 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.29801 HOMO: -6.29399 LUMO: 0.06803 factor:1 | 1 (-1.75968) | -1 | -1 |
| G: -6257.17264 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.50041 HOMO: -6.60692 LUMO: -0.47076 factor:1 | 1 (-1.96208) | -1 | -1 |
| G: -6257.17264 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.91244 HOMO: -7.33891 LUMO: 0.39184 factor:1 | 1 (-2.37411) | 1 | 1 |
| G: -6257.17264 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.50199 HOMO: -6.60692 LUMO: 1.46125 factor:1 | 1 (-1.96366) | -1 | -1 |
| G: -6257.17264 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12524.04134 HOMO: -6.21780 LUMO: 2.09256 factor:1 | 1 (-2.50301) | -1 | -1 |
| G: -6257.17264 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.30005 HOMO: -6.28311 LUMO: 1.80411 factor:1 | 1 (-1.76172) | -1 | -1 |
| G: -6257.17264 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.79747 HOMO: -6.51168 LUMO: 1.84765 factor:1 | 1 (-2.25914) | -1 | -1 |
| G: -6257.17264 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.84050 HOMO: -6.66951 LUMO: 2.01636 factor:1 | 1 (-2.30216) | -1 | -1 |
| G: -6257.17264 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12524.12725 HOMO: -6.75387 LUMO: 1.73881 factor:1 | 1 (-2.58892) | -1 | -1 |
| G: -6257.17264 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.90270 HOMO: -6.77291 LUMO: 1.89935 factor:1 | 1 (-2.36437) | -1 | -1 |
| G: -6257.17264 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.23512 HOMO: -6.36474 LUMO: 1.61091 factor:1 | 1 (-1.69679) | -1 | -1 |
| G: -6257.17264 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.72558 HOMO: -6.60420 LUMO: 1.40955 factor:1 | 1 (-2.18725) | -1 | -1 |
| G: -6257.17264 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.48778 HOMO: -6.81645 LUMO: 1.59731 factor:1 | 1 (-1.94945) | -1 | -1 |
| G: -6257.17264 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.29659 HOMO: -5.90215 LUMO: 2.12249 factor:1 | 1 (-1.75826) | -1 | -1 |
| G: -6257.17264 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.42117 HOMO: -6.26950 LUMO: 1.62996 factor:1 | 1 (-1.88284) | -1 | -1 |
| G: -6257.17264 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.30571 HOMO: -6.41100 LUMO: 1.80684 factor:1 | 1 (-1.76738) | -1 | -1 |
| G: -6257.17264 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.96056 HOMO: -6.64230 LUMO: 2.23405 factor:1 | 1 (-1.42223) | -1 | -1 |
| G: -6257.17264 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.10065 HOMO: -6.66951 LUMO: 2.21501 factor:1 | 1 (-1.56231) | -1 | -1 |
| G: -6257.17264 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.11431 HOMO: -6.90897 LUMO: 2.00004 factor:1 | 1 (-1.57597) | -1 | -1 |
| G: -6257.17264 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.15066 HOMO: -6.61781 LUMO: 1.42043 factor:1 | 1 (-1.61233) | -1 | -1 |
| G: -6257.17264 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.20723 HOMO: -6.56611 LUMO: 1.60003 factor:1 | 1 (-1.66890) | -1 | -1 |
| G: -6257.17264 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.23654 HOMO: -6.70489 LUMO: 1.78779 factor:1 | 1 (-1.69821) | -1 | -1 |
| G: -6257.17264 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12524.00091 HOMO: -6.46815 LUMO: 1.59459 factor:1 | 1 (-2.46258) | -1 | -1 |
| G: -6257.17264 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.73165 HOMO: -6.31304 LUMO: 1.36873 factor:1 | 1 (-2.19332) | -1 | -1 |
| G: -6257.17264 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.96580 HOMO: -6.22597 LUMO: 1.54833 factor:1 | 1 (-2.42747) | -1 | -1 |
| G: -6257.17264 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.25042 HOMO: -5.63004 LUMO: 1.96466 factor:1 | 1 (-1.71209) | -1 | -1 |
| G: -6257.17264 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.34876 HOMO: -7.02598 LUMO: 1.79323 factor:1 | 1 (-1.81043) | -1 | -1 |
| G: -6257.17264 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.92528 HOMO: -6.78924 LUMO: 2.10888 factor:1 | 1 (-0.38695) | -1 | -1 |
| G: -6257.17264 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.04046 HOMO: -6.13345 LUMO: 2.07351 factor:1 | 1 (-0.50213) | -1 | -1 |
| G: -6257.17264 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.79136 HOMO: -6.46270 LUMO: -0.37552 factor:1 | 1 (-1.25303) | -1 | -1 |
| G: -6257.17264 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.87267 HOMO: -6.51985 LUMO: -0.49525 factor:1 | 1 (-1.33434) | -1 | -1 |
| G: -6257.17264 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.15334 HOMO: -6.60965 LUMO: 1.90480 factor:1 | 1 (-0.61500) | -1 | -1 |
| G: -6257.17264 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.30003 HOMO: -6.51168 LUMO: 1.92112 factor:1 | 1 (-0.76170) | -1 | -1 |
| G: -6257.17264 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.25678 HOMO: -6.71305 LUMO: 1.91024 factor:1 | 1 (-1.71845) | -1 | -1 |
| G: -6257.17264 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.21970 HOMO: -6.86815 LUMO: 2.02997 factor:1 | 1 (-1.68136) | -1 | -1 |
| G: -6257.17264 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.29034 HOMO: -6.69944 LUMO: 1.95106 factor:1 | 1 (-1.75201) | -1 | -1 |
| G: -6257.17264 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.92988 HOMO: -6.45182 LUMO: 1.66806 factor:1 | 1 (-0.39154) | -1 | -1 |
| G: -6257.17264 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.06490 HOMO: -6.44638 LUMO: 2.16058 factor:1 | 1 (-0.52657) | -1 | -1 |
| G: -6257.17264 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.86846 HOMO: -6.65591 LUMO: 1.95106 factor:1 | 1 (-0.33013) | -1 | -1 |
| G: -6257.17264 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.83781 HOMO: -6.35114 LUMO: 1.42316 factor:1 | 1 (-1.29948) | -1 | -1 |
| G: -6257.17264 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.76807 HOMO: -6.48719 LUMO: 1.59187 factor:1 | 1 (-1.22974) | -1 | -1 |
| G: -6257.17264 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.90227 HOMO: -7.05591 LUMO: 1.61908 factor:1 | 1 (-1.36394) | -1 | -1 |
| G: -6257.17264 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.02304 HOMO: -6.92258 LUMO: 1.87214 factor:1 | 1 (-1.48471) | -1 | -1 |
| G: -6257.17264 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.79120 HOMO: -5.85861 LUMO: 2.11705 factor:1 | 1 (-1.25287) | -1 | -1 |
| G: -6257.17264 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.83381 HOMO: -6.27767 LUMO: 1.75513 factor:1 | 1 (-1.29548) | -1 | -1 |
| G: -6257.17264 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.99351 HOMO: -6.16882 LUMO: 1.73881 factor:1 | 1 (-1.45518) | -1 | -1 |
| G: -6257.17264 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.92878 HOMO: -6.62053 LUMO: 1.39594 factor:1 | 1 (-1.39045) | -1 | -1 |
| G: -6257.17264 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.53137 HOMO: -5.46405 LUMO: 1.68166 factor:1 | 1 (-1.99304) | -1 | -1 |
| G: -6257.17264 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.86368 HOMO: -6.39740 LUMO: 1.68711 factor:1 | 1 (-2.32535) | -1 | -1 |
| G: -6257.17264 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.73358 HOMO: -6.99333 LUMO: 2.08439 factor:1 | 1 (-2.19525) | -1 | -1 |
| G: -6257.17264 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.06429 HOMO: -6.16882 LUMO: 1.71976 factor:1 | 1 (-1.52596) | -1 | -1 |
| G: -6257.17264 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.08701 HOMO: -7.19741 LUMO: 2.24766 factor:1 | 1 (-1.54868) | 1 | 1 |
| G: -6257.17264 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.58389 HOMO: -6.77291 LUMO: 2.17691 factor:1 | 1 (-2.04556) | -1 | -1 |
| G: -6257.17264 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.88110 HOMO: -6.29944 LUMO: 2.16603 factor:1 | 1 (-1.34277) | -1 | -1 |
| G: -6257.17264 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.73476 HOMO: -6.10079 LUMO: 1.83949 factor:1 | 1 (-1.19643) | -1 | -1 |
| G: -6257.17264 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.80453 HOMO: -6.63686 LUMO: 2.05990 factor:1 | 1 (-1.26620) | -1 | -1 |
| G: -6257.17264 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.60711 HOMO: -6.91713 LUMO: 1.87486 factor:1 | 1 (-1.06878) | -1 | -1 |
| G: -6257.17264 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.35204 HOMO: -6.63958 LUMO: 1.79323 factor:1 | -1 (0.18629) | -1 | -1 |
| G: -6257.17264 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.27784 HOMO: -6.61781 LUMO: 1.70071 factor:1 | -1 (0.26049) | -1 | -1 |
| G: -6257.17264 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.56007 HOMO: -6.20420 LUMO: 1.82861 factor:1 | 1 (-0.02174) | -1 | -1 |
| G: -6257.17264 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.30390 HOMO: -6.47903 LUMO: -2.16875 factor:1 | 1 (-0.76557) | -1 | -1 |
| G: -6257.17264 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.99030 HOMO: -6.53073 LUMO: 2.18235 factor:1 | 1 (-1.45197) | -1 | -1 |
| G: -6257.17264 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.81920 HOMO: -7.01782 LUMO: 1.72520 factor:1 | 1 (-1.28087) | -1 | -1 |
| G: -6257.17264 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.45037 HOMO: -6.66135 LUMO: -0.75648 factor:1 | 1 (-0.91204) | -1 | -1 |
| G: -6257.17264 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.48303 HOMO: -7.56749 LUMO: 0.22585 factor:1 | 1 (-0.94470) | 1 | 1 |
| G: -6257.17264 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.45427 HOMO: -6.45182 LUMO: -0.71294 factor:1 | -1 (0.08406) | -1 | -1 |
| G: -6257.17264 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.45193 HOMO: -6.31032 LUMO: -0.34286 factor:1 | -1 (0.08640) | -1 | -1 |
| G: -6257.17264 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.58043 HOMO: -6.41917 LUMO: 2.04085 factor:1 | 1 (-0.04210) | -1 | -1 |
| G: -6257.17264 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.03197 HOMO: -6.61781 LUMO: 1.98915 factor:1 | 1 (-0.49364) | -1 | -1 |
| G: -6257.17264 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.14082 HOMO: -5.86405 LUMO: 1.57282 factor:1 | 1 (-0.60249) | -1 | -1 |
| G: -6257.17264 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.98449 HOMO: -6.44094 LUMO: 1.80956 factor:1 | 1 (-0.44616) | -1 | -1 |
| G: -6257.17264 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.47262 HOMO: -6.59060 LUMO: 2.08167 factor:1 | -1 (0.06572) | -1 | -1 |
| G: -6257.17264 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.50034 HOMO: -6.20147 LUMO: 1.69799 factor:1 | -1 (0.03799) | -1 | -1 |
| G: -6257.17264 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.41215 HOMO: -6.50352 LUMO: -0.41361 factor:1 | -1 (0.12618) | -1 | -1 |
| G: -6257.17264 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.10246 HOMO: -6.10896 LUMO: -0.55783 factor:1 | -1 (0.43587) | -1 | -1 |
| G: -6257.17264 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.52395 HOMO: -6.74842 LUMO: -0.56872 factor:1 | 1 (-0.98562) | -1 | -1 |
| G: -6257.17264 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.33709 HOMO: -6.59060 LUMO: -0.22041 factor:1 | 1 (-1.79875) | -1 | -1 |
| G: -6257.17264 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.26326 HOMO: -6.22052 LUMO: -0.60137 factor:1 | 1 (-1.72493) | -1 | -1 |
| G: -6257.17264 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.17261 HOMO: -6.65863 LUMO: 0.07891 factor:1 | -1 (0.36572) | -1 | -1 |
| G: -6257.17264 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.65367 HOMO: -6.57427 LUMO: 1.71160 factor:1 | 1 (-1.11534) | -1 | -1 |
| G: -6257.17264 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.65830 HOMO: -5.84773 LUMO: 1.99459 factor:1 | 1 (-1.11997) | -1 | -1 |
| G: -6257.17264 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.97205 HOMO: -6.02188 LUMO: 1.91296 factor:1 | 1 (-0.43372) | -1 | -1 |
| G: -6257.17264 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.75718 HOMO: -6.17698 LUMO: 2.00004 factor:1 | 1 (-1.21885) | -1 | -1 |
| G: -6257.17264 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.07176 HOMO: -6.02732 LUMO: 1.90752 factor:1 | 1 (-0.53342) | -1 | -1 |
| G: -6257.17264 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.18104 HOMO: -6.68584 LUMO: -0.50885 factor:1 | 1 (-0.64271) | -1 | -1 |
| G: -6257.17264 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.16109 HOMO: -6.61781 LUMO: -0.73471 factor:1 | 1 (-0.62276) | -1 | -1 |
| G: -6257.17264 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.16476 HOMO: -6.66407 LUMO: -0.79729 factor:1 | 1 (-0.62643) | -1 | -1 |
| G: -6257.17264 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.26278 HOMO: -6.56339 LUMO: 0.23130 factor:1 | 1 (-0.72445) | -1 | -1 |
| G: -6257.17264 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.13875 HOMO: -6.76747 LUMO: 0.08980 factor:1 | 1 (-0.60042) | -1 | -1 |
| G: -6257.17264 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.04691 HOMO: -6.70489 LUMO: -0.53334 factor:1 | 1 (-0.50858) | -1 | -1 |
| G: -6257.17264 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.14016 HOMO: -7.28993 LUMO: 0.10885 factor:1 | 1 (-0.60183) | 1 | 1 |
| G: -6257.17264 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.12095 HOMO: -6.22052 LUMO: 0.51974 factor:1 | 1 (-0.58262) | -1 | -1 |
| G: -6257.17264 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.05502 HOMO: -6.81645 LUMO: 0.25307 factor:1 | 1 (-0.51669) | -1 | -1 |
| G: -6257.17264 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.26006 HOMO: -6.80285 LUMO: 0.02721 factor:1 | 1 (-0.72173) | -1 | -1 |
| G: -6257.17264 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.05350 HOMO: -6.51441 LUMO: 0.08163 factor:1 | 1 (-0.51517) | -1 | -1 |
| G: -6257.17264 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.08523 HOMO: -6.73482 LUMO: -0.77008 factor:1 | 1 (-0.54689) | -1 | -1 |
| G: -6257.17264 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.09777 HOMO: -6.29127 LUMO: -0.44355 factor:1 | 1 (-0.55944) | -1 | -1 |
| G: -6257.17264 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.94922 HOMO: -6.72938 LUMO: -0.64763 factor:1 | 1 (-0.41089) | -1 | -1 |
| G: -6257.17264 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.82302 HOMO: -6.49264 LUMO: -0.74559 factor:1 | 1 (-0.28469) | -1 | -1 |
| G: -6257.17264 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.04746 HOMO: -6.67223 LUMO: -0.55239 factor:1 | 1 (-0.50913) | -1 | -1 |
| G: -6257.17264 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.82310 HOMO: -6.33481 LUMO: 0.33198 factor:1 | 1 (-0.28477) | -1 | -1 |
| G: -6257.17264 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.14226 HOMO: -6.76475 LUMO: -0.25307 factor:1 | 1 (-0.60393) | -1 | -1 |
| G: -6257.17264 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.42232 HOMO: -6.65318 LUMO: 0.03810 factor:1 | 1 (-0.88399) | -1 | -1 |
| G: -6257.17264 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.99584 HOMO: -6.09263 LUMO: 0.21497 factor:1 | 1 (-0.45751) | -1 | -1 |
| G: -6257.17264 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.99858 HOMO: -6.32120 LUMO: -0.85444 factor:1 | 1 (-0.46025) | -1 | -1 |
| G: -6257.17264 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.69120 HOMO: -6.57155 LUMO: -0.67484 factor:1 | 1 (-0.15287) | -1 | -1 |
| G: -6257.17264 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.04898 HOMO: -6.53345 LUMO: -0.78913 factor:1 | 1 (-0.51065) | -1 | -1 |
| G: -6257.17264 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.10950 HOMO: -7.07768 LUMO: 0.28844 factor:1 | 1 (-0.57117) | 1 | 1 |
| G: -6257.17264 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.25317 HOMO: -6.75114 LUMO: 0.18776 factor:1 | 1 (-0.71484) | -1 | -1 |
| G: -6257.17264 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.12248 HOMO: -6.77019 LUMO: -0.12245 factor:1 | 1 (-0.58415) | -1 | -1 |
| G: -6257.17264 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.68709 HOMO: -6.43549 LUMO: 0.16327 factor:1 | 1 (-1.14876) | -1 | -1 |
| G: -6257.17264 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.67615 HOMO: -6.69400 LUMO: -0.16327 factor:1 | 1 (-1.13782) | -1 | -1 |
| G: -6257.17264 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.95093 HOMO: -6.38651 LUMO: -0.61770 factor:1 | 1 (-1.41260) | -1 | -1 |
| G: -6257.17264 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.95422 HOMO: -6.34297 LUMO: -0.33198 factor:1 | 1 (-1.41589) | -1 | -1 |
| G: -6257.17264 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.80363 HOMO: -7.51578 LUMO: 0.02177 factor:1 | 1 (-1.26530) | 1 | 1 |
| G: -6257.17264 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.94010 HOMO: -6.47359 LUMO: -0.22585 factor:1 | 1 (-1.40177) | -1 | -1 |
| G: -6257.17264 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.53753 HOMO: -6.68040 LUMO: -0.47076 factor:1 | 1 (-0.99920) | -1 | -1 |
| G: -6257.17264 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.10596 HOMO: -6.75659 LUMO: -0.57688 factor:1 | 1 (-0.56763) | -1 | -1 |
| G: -6257.17264 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.01905 HOMO: -6.73754 LUMO: -0.61226 factor:1 | 1 (-0.48072) | -1 | -1 |
| G: -6257.17264 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.64907 HOMO: -7.37429 LUMO: 0.31293 factor:1 | 1 (-1.11074) | 1 | 1 |
| G: -6257.17264 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.71925 HOMO: -6.23413 LUMO: -0.90886 factor:1 | 1 (-1.18092) | -1 | -1 |
| G: -6257.17264 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.78200 HOMO: -6.51985 LUMO: -0.68028 factor:1 | 1 (-1.24367) | -1 | -1 |
| G: -6257.17264 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.50937 HOMO: -6.52257 LUMO: -0.77280 factor:1 | 1 (-0.97104) | -1 | -1 |
| G: -6257.17264 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.87297 HOMO: -7.29537 LUMO: 0.31837 factor:1 | 1 (-1.33464) | 1 | 1 |
| G: -6257.17264 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.72702 HOMO: -6.08447 LUMO: 0.25851 factor:1 | 1 (-2.18869) | -1 | -1 |
| G: -6257.17264 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.13624 HOMO: -6.20964 LUMO: 0.13606 factor:1 | 1 (-1.59791) | -1 | -1 |
| G: -6257.17264 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.75655 HOMO: -6.49808 LUMO: -0.14150 factor:1 | 1 (-2.21822) | -1 | -1 |
| G: -6257.17264 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.00075 HOMO: -7.10761 LUMO: 0.28028 factor:1 | 1 (-1.46242) | 1 | 1 |
| G: -6257.17264 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.17031 HOMO: -6.60965 LUMO: -0.62858 factor:1 | 1 (-1.63198) | -1 | -1 |
| G: -6257.17264 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.79415 HOMO: -6.40012 LUMO: -0.26939 factor:1 | 1 (-2.25582) | -1 | -1 |
| G: -6257.17264 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.39894 HOMO: -6.65318 LUMO: -0.73199 factor:1 | 1 (-1.86061) | -1 | -1 |
| G: -6257.17264 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.78569 HOMO: -6.51441 LUMO: -0.44899 factor:1 | 1 (-2.24736) | -1 | -1 |
| G: -6257.17264 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.48101 HOMO: -6.28583 LUMO: -0.48708 factor:1 | 1 (-1.94268) | -1 | -1 |
| G: -6257.17264 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.75611 HOMO: -6.96884 LUMO: 0.19864 factor:1 | 1 (-2.21778) | -1 | -1 |
| G: -6257.17264 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.58561 HOMO: -6.89809 LUMO: 0.34558 factor:1 | 1 (-2.04728) | -1 | -1 |
| G: -6257.17264 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.84445 HOMO: -6.67495 LUMO: -0.15510 factor:1 | 1 (-1.30612) | -1 | -1 |
| G: -6257.17264 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.35355 HOMO: -7.34980 LUMO: 0.19864 factor:1 | 1 (-1.81522) | 1 | 1 |
| G: -6257.17264 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.95860 HOMO: -6.71305 LUMO: -0.81634 factor:1 | 1 (-1.42027) | -1 | -1 |
| G: -6257.17264 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.99852 HOMO: -6.39468 LUMO: -0.47076 factor:1 | 1 (-1.46019) | -1 | -1 |
| G: -6257.17264 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.40917 HOMO: -6.31304 LUMO: 1.39594 factor:1 | 1 (-1.87084) | -1 | -1 |
| G: -6257.17264 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.53524 HOMO: -6.57155 LUMO: 1.55105 factor:1 | 1 (-1.99691) | -1 | -1 |
| G: -6257.17264 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.31306 HOMO: -6.68312 LUMO: 1.69255 factor:1 | 1 (-1.77473) | -1 | -1 |
| G: -6257.17264 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.30677 HOMO: -6.61509 LUMO: 1.73881 factor:1 | 1 (-1.76844) | -1 | -1 |
| G: -6257.17264 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.20693 HOMO: -6.17971 LUMO: 1.90208 factor:1 | 1 (-1.66860) | -1 | -1 |
| G: -6257.17264 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.60982 HOMO: -6.53073 LUMO: 1.73337 factor:1 | 1 (-2.07149) | -1 | -1 |
| G: -6257.17264 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.13178 HOMO: -5.91303 LUMO: 1.90480 factor:1 | 1 (-0.59345) | -1 | -1 |
| G: -6257.17264 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.89694 HOMO: -6.42733 LUMO: 1.80139 factor:1 | 1 (-1.35861) | -1 | -1 |
| G: -6257.17264 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.87207 HOMO: -6.78924 LUMO: 2.31569 factor:1 | 1 (-1.33374) | -1 | -1 |
| G: -6257.17264 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.70935 HOMO: -6.04093 LUMO: 1.91568 factor:1 | 1 (-1.17101) | -1 | -1 |
| G: -6257.17264 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.99006 HOMO: -6.90081 LUMO: 2.36739 factor:1 | 1 (-1.45173) | -1 | -1 |
| G: -6257.17264 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.94832 HOMO: -6.60965 LUMO: 2.18507 factor:1 | 1 (-1.40999) | -1 | -1 |
| G: -6257.17264 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.87928 HOMO: -6.75387 LUMO: 2.48712 factor:1 | 1 (-1.34095) | -1 | -1 |
| G: -6257.17264 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.75590 HOMO: -6.56883 LUMO: 1.71432 factor:1 | 1 (-1.21757) | -1 | -1 |
| G: -6257.17264 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.98467 HOMO: -6.41644 LUMO: 1.72792 factor:1 | 1 (-1.44634) | -1 | -1 |
| G: -6257.17264 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.88630 HOMO: -6.92530 LUMO: 2.54426 factor:1 | 1 (-1.34797) | -1 | -1 |
| G: -6257.17264 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.97060 HOMO: -6.41644 LUMO: 2.70209 factor:1 | 1 (-1.43227) | -1 | -1 |
| G: -6257.17264 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.97213 HOMO: -6.29671 LUMO: 2.14698 factor:1 | 1 (-1.43380) | -1 | -1 |
| G: -6257.17264 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.13069 HOMO: -6.29127 LUMO: 1.87486 factor:1 | 1 (-1.59236) | -1 | -1 |
| G: -6257.17264 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.94949 HOMO: -6.75931 LUMO: 2.78917 factor:1 | 1 (-0.41116) | -1 | -1 |
| G: -6257.17264 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.88732 HOMO: -6.40828 LUMO: 1.86942 factor:1 | 1 (-0.34899) | -1 | -1 |
| G: -6257.17264 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.90658 HOMO: -6.45726 LUMO: 1.97010 factor:1 | 1 (-0.36825) | -1 | -1 |
| G: -6257.17264 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.74620 HOMO: -6.43277 LUMO: 1.22723 factor:1 | 1 (-0.20787) | -1 | -1 |
| G: -6257.17264 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.11738 HOMO: -6.63414 LUMO: 1.62452 factor:1 | 1 (-1.57905) | -1 | -1 |
| G: -6257.17264 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.19409 HOMO: -6.54162 LUMO: 2.16058 factor:1 | 1 (-1.65576) | -1 | -1 |
| G: -6257.17264 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.10486 HOMO: -6.40284 LUMO: 1.88575 factor:1 | 1 (-1.56653) | -1 | -1 |
| G: -6257.17264 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.85483 HOMO: -6.20964 LUMO: 1.84221 factor:1 | 1 (-0.31650) | -1 | -1 |
| G: -6257.17264 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.91815 HOMO: -6.58516 LUMO: 1.69799 factor:1 | 1 (-0.37982) | -1 | -1 |
| G: -6257.17264 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.72906 HOMO: -6.44094 LUMO: 2.05446 factor:1 | 1 (-0.19072) | -1 | -1 |
| G: -6257.17264 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.72800 HOMO: -6.61509 LUMO: 2.16058 factor:1 | 1 (-2.18967) | -1 | -1 |
| G: -6257.17264 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.38343 HOMO: -6.65591 LUMO: 1.69527 factor:1 | 1 (-1.84510) | -1 | -1 |
| G: -6257.17264 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.48264 HOMO: -5.55112 LUMO: 1.80411 factor:1 | 1 (-1.94431) | -1 | -1 |
| G: -6257.17264 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.89912 HOMO: -6.68312 LUMO: 2.38100 factor:1 | 1 (-1.36079) | -1 | -1 |
| G: -6257.17264 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.61325 HOMO: -6.51168 LUMO: 2.14698 factor:1 | 1 (-2.07492) | -1 | -1 |
| G: -6257.17264 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.87384 HOMO: -6.04637 LUMO: 1.48302 factor:1 | 1 (-1.33551) | -1 | -1 |
| G: -6257.17264 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.74733 HOMO: -6.81645 LUMO: -0.74287 factor:1 | 1 (-1.20900) | -1 | -1 |
| G: -6257.17264 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.09597 HOMO: -6.96884 LUMO: -0.97961 factor:1 | 1 (-0.55764) | -1 | -1 |
| G: -6257.17264 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.98612 HOMO: -6.45998 LUMO: 0.09796 factor:1 | 1 (-0.44779) | -1 | -1 |
| G: -6257.17264 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.95616 HOMO: -6.44638 LUMO: 0.09524 factor:1 | 1 (-0.41783) | -1 | -1 |
| G: -6257.17264 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.11720 HOMO: -6.16338 LUMO: -0.54151 factor:1 | 1 (-0.57887) | -1 | -1 |
| G: -6257.17264 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.04441 HOMO: -6.35930 LUMO: -0.47892 factor:1 | 1 (-0.50608) | -1 | -1 |
| G: -6257.17264 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.98501 HOMO: -6.65318 LUMO: -0.00272 factor:1 | 1 (-0.44667) | -1 | -1 |
| G: -6257.17264 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.96228 HOMO: -6.50080 LUMO: 0.14694 factor:1 | 1 (-0.42395) | -1 | -1 |
| G: -6257.17264 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.95798 HOMO: -6.60420 LUMO: 0.94968 factor:1 | 1 (-0.41965) | -1 | -1 |
| G: -6257.17264 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.77390 HOMO: -6.60148 LUMO: -0.77552 factor:1 | 1 (-0.23557) | -1 | -1 |
| G: -6257.17264 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.01303 HOMO: -6.81645 LUMO: -1.05580 factor:1 | 1 (-0.47470) | -1 | -1 |
| G: -6257.17264 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.99118 HOMO: -6.57971 LUMO: -0.82178 factor:1 | 1 (-0.45285) | -1 | -1 |
| G: -6257.17264 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.72486 HOMO: -6.09263 LUMO: -0.45171 factor:1 | 1 (-0.18653) | -1 | -1 |
| G: -6257.17264 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.79600 HOMO: -6.74298 LUMO: -0.61770 factor:1 | 1 (-0.25766) | -1 | -1 |
| G: -6257.17264 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.16248 HOMO: -6.72393 LUMO: 1.21091 factor:1 | 1 (-0.62415) | -1 | -1 |
| G: -6257.17264 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.05085 HOMO: -6.30488 LUMO: 1.70071 factor:1 | 1 (-1.51252) | -1 | -1 |
| G: -6257.17264 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.58670 HOMO: -6.38107 LUMO: 1.55649 factor:1 | 1 (-2.04836) | -1 | -1 |
| G: -6257.17264 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.88254 HOMO: -6.17154 LUMO: 1.46669 factor:1 | 1 (-2.34421) | -1 | -1 |
| G: -6257.17264 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.42392 HOMO: -6.86543 LUMO: 1.98643 factor:1 | 1 (-1.88559) | -1 | -1 |
| G: -6257.17264 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.31314 HOMO: -6.69944 LUMO: 1.65173 factor:1 | 1 (-1.77481) | -1 | -1 |
| G: -6257.17264 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.65973 HOMO: -6.77836 LUMO: 2.16331 factor:1 | 1 (-2.12140) | -1 | -1 |
| G: -6257.17264 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.68512 HOMO: -6.42189 LUMO: 2.36467 factor:1 | 1 (-2.14679) | -1 | -1 |
| G: -6257.17264 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.68901 HOMO: -7.00965 LUMO: 2.04358 factor:1 | 1 (-2.15068) | -1 | -1 |
| G: -6257.17264 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.00448 HOMO: -6.36746 LUMO: 2.13881 factor:1 | 1 (-1.46615) | -1 | -1 |
| G: -6257.17264 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.97814 HOMO: -6.37835 LUMO: 1.89935 factor:1 | 1 (-1.43981) | -1 | -1 |
| G: -6257.17264 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.96403 HOMO: -7.03959 LUMO: 1.27349 factor:1 | 1 (-0.42569) | -1 | -1 |
| G: -6257.17264 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.91355 HOMO: -6.67495 LUMO: -0.89253 factor:1 | 1 (-0.37522) | -1 | -1 |
| G: -6257.17264 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.04811 HOMO: -6.71849 LUMO: -0.97961 factor:1 | 1 (-0.50978) | -1 | -1 |
| G: -6257.17264 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.06512 HOMO: -6.47903 LUMO: 0.01633 factor:1 | 1 (-0.52679) | -1 | -1 |
| G: -6257.17264 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.83678 HOMO: -6.38379 LUMO: 0.01088 factor:1 | 1 (-1.29845) | -1 | -1 |
| G: -6257.17264 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.62485 HOMO: -6.49536 LUMO: -0.55239 factor:1 | 1 (-1.08652) | -1 | -1 |
| G: -6257.17264 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.91931 HOMO: -6.53345 LUMO: -0.53879 factor:1 | 1 (-1.38098) | -1 | -1 |
| G: -6257.17264 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.87104 HOMO: -6.16610 LUMO: 2.15514 factor:1 | 1 (-1.33270) | -1 | -1 |
| G: -6257.17264 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.83743 HOMO: -6.35114 LUMO: 1.98643 factor:1 | 1 (-1.29910) | -1 | -1 |
| G: -6257.17264 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.89446 HOMO: -6.43277 LUMO: 2.16058 factor:1 | 1 (-1.35613) | -1 | -1 |
| G: -6257.17264 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.90381 HOMO: -6.89809 LUMO: 2.20684 factor:1 | 1 (-0.36548) | -1 | -1 |
| G: -6257.17264 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.64742 HOMO: -6.54434 LUMO: 1.93473 factor:1 | 1 (-0.10909) | -1 | -1 |
| G: -6257.17264 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.75458 HOMO: -6.72938 LUMO: 2.03269 factor:1 | 1 (-0.21625) | -1 | -1 |
| G: -6257.17264 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.92993 HOMO: -6.90353 LUMO: 2.19868 factor:1 | 1 (-0.39160) | -1 | -1 |
| G: -6257.17264 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.65448 HOMO: -6.41372 LUMO: 2.02453 factor:1 | 1 (-2.11615) | -1 | -1 |
| G: -6257.17264 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.20467 HOMO: -6.46543 LUMO: 1.90752 factor:1 | 1 (-1.66634) | -1 | -1 |
| G: -6257.17264 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.76409 HOMO: -6.55522 LUMO: 2.11977 factor:1 | 1 (-1.22576) | -1 | -1 |
| G: -6257.17264 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.47325 HOMO: -6.28855 LUMO: 2.02181 factor:1 | 1 (-1.93492) | -1 | -1 |
| G: -6257.17264 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.72151 HOMO: -6.45726 LUMO: 1.52112 factor:1 | 1 (-1.18318) | -1 | -1 |
| G: -6257.17264 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.05779 HOMO: -6.37291 LUMO: 2.11705 factor:1 | 1 (-1.51946) | -1 | -1 |
| G: -6257.17264 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.51562 HOMO: -6.88448 LUMO: 2.24494 factor:1 | 1 (-1.97729) | -1 | -1 |
| G: -6257.17264 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.14318 HOMO: -6.86271 LUMO: 2.41637 factor:1 | 1 (-1.60485) | -1 | -1 |
| G: -6257.17264 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.15948 HOMO: -6.69400 LUMO: 2.34562 factor:1 | 1 (-1.62115) | -1 | -1 |
| G: -6257.17264 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.88807 HOMO: -6.18243 LUMO: 2.53882 factor:1 | 1 (-1.34974) | -1 | -1 |
| G: -6257.17264 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.89075 HOMO: -6.61237 LUMO: 2.54154 factor:1 | 1 (-0.35241) | -1 | -1 |
| G: -6257.17264 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.53028 HOMO: -6.69672 LUMO: 2.16331 factor:1 | -1 (0.00805) | -1 | -1 |
| G: -6257.17264 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.44627 HOMO: -6.33481 LUMO: 2.34018 factor:1 | -1 (0.09206) | -1 | -1 |
| G: -6257.17264 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.15560 HOMO: -5.99739 LUMO: 2.37283 factor:1 | -1 (0.38273) | -1 | -1 |
| G: -6257.17264 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.33542 HOMO: -6.49808 LUMO: 2.47351 factor:1 | -1 (0.20292) | -1 | -1 |
| G: -6257.17264 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.44355 HOMO: -6.22052 LUMO: 1.86398 factor:1 | -1 (0.09478) | -1 | -1 |
| G: -6257.17264 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.52435 HOMO: -6.32665 LUMO: 2.28031 factor:1 | 1 (-1.98602) | -1 | -1 |
| G: -6257.17264 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.66604 HOMO: -5.98378 LUMO: 2.16331 factor:1 | 1 (-2.12771) | -1 | -1 |
| G: -6257.17264 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12524.00349 HOMO: -6.08991 LUMO: 2.30208 factor:1 | 1 (-2.46516) | -1 | -1 |
| G: -6257.17264 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.37047 HOMO: -7.07224 LUMO: 1.55105 factor:1 | 1 (-1.83214) | 1 | 1 |
| G: -6257.17264 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.63285 HOMO: -6.84638 LUMO: 1.76874 factor:1 | 1 (-2.09451) | -1 | -1 |
| G: -6257.17264 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.95051 HOMO: -6.68856 LUMO: 1.47758 factor:1 | 1 (-2.41218) | -1 | -1 |
| G: -6257.17264 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.65374 HOMO: -6.69672 LUMO: 1.71976 factor:1 | 1 (-2.11541) | -1 | -1 |
| G: -6257.17264 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.90352 HOMO: -6.86543 LUMO: 2.24766 factor:1 | 1 (-2.36519) | -1 | -1 |
| G: -6257.17264 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12524.26777 HOMO: -7.21646 LUMO: 1.71976 factor:1 | 1 (-2.72944) | 1 | 1 |
| G: -6257.17264 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.39320 HOMO: -6.94162 LUMO: 2.21773 factor:1 | 1 (-0.85487) | -1 | -1 |
| G: -6257.17264 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.47008 HOMO: -6.34842 LUMO: 2.04358 factor:1 | 1 (-0.93175) | -1 | -1 |
| G: -6257.17264 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.97289 HOMO: -6.53345 LUMO: 1.96738 factor:1 | 1 (-1.43456) | -1 | -1 |
| G: -6257.17264 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.05621 HOMO: -6.34842 LUMO: 1.88303 factor:1 | 1 (-1.51788) | -1 | -1 |
| G: -6257.17264 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.49350 HOMO: -6.38651 LUMO: 2.08983 factor:1 | 1 (-0.95517) | -1 | -1 |
| G: -6257.17264 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.36498 HOMO: -6.01372 LUMO: 1.43676 factor:1 | 1 (-1.82665) | -1 | -1 |
| G: -6257.17264 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.99974 HOMO: -6.30216 LUMO: 1.41771 factor:1 | 1 (-2.46141) | -1 | -1 |
| G: -6257.17264 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.51437 HOMO: -6.52801 LUMO: 1.77146 factor:1 | 1 (-1.97604) | -1 | -1 |
| G: -6257.17264 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.95623 HOMO: -6.53617 LUMO: 1.72792 factor:1 | 1 (-2.41789) | -1 | -1 |
| G: -6257.17264 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.62224 HOMO: -6.56611 LUMO: 2.20412 factor:1 | 1 (-1.08391) | -1 | -1 |
| G: -6257.17264 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.45437 HOMO: -6.66679 LUMO: -0.72927 factor:1 | 1 (-0.91604) | -1 | -1 |
| G: -6257.17264 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.46627 HOMO: -6.85455 LUMO: -0.85444 factor:1 | 1 (-0.92794) | -1 | -1 |
| G: -6257.17264 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.74042 HOMO: -7.21646 LUMO: 0.27211 factor:1 | 1 (-1.20209) | 1 | 1 |
| G: -6257.17264 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.26157 HOMO: -6.57971 LUMO: -0.41361 factor:1 | 1 (-1.72324) | -1 | -1 |
| G: -6257.17264 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.18614 HOMO: -7.03142 LUMO: -1.14288 factor:1 | 1 (-1.64781) | -1 | -1 |
| G: -6257.17264 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.17474 HOMO: -6.29944 LUMO: 0.06803 factor:1 | 1 (-1.63641) | -1 | -1 |
| G: -6257.17264 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.58066 HOMO: -6.47359 LUMO: 0.28028 factor:1 | 1 (-1.04233) | -1 | -1 |
| G: -6257.17264 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.31892 HOMO: -6.42189 LUMO: 1.61364 factor:1 | 1 (-0.78059) | -1 | -1 |
| G: -6257.17264 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.46289 HOMO: -6.41100 LUMO: 1.80956 factor:1 | 1 (-0.92456) | -1 | -1 |
| G: -6257.17264 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.05972 HOMO: -6.83278 LUMO: 1.83949 factor:1 | 1 (-1.52139) | -1 | -1 |
| G: -6257.17264 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.94108 HOMO: -6.78380 LUMO: -0.76192 factor:1 | 1 (-1.40275) | -1 | -1 |
| G: -6257.17264 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.19684 HOMO: -6.95795 LUMO: 2.13609 factor:1 | 1 (-1.65851) | -1 | -1 |
| G: -6257.17264 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.65122 HOMO: -6.57155 LUMO: 1.89119 factor:1 | 1 (-1.11289) | -1 | -1 |
| G: -6257.17264 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.48335 HOMO: -6.65591 LUMO: 1.93745 factor:1 | 1 (-0.94502) | -1 | -1 |
| G: -6257.17264 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.27826 HOMO: -6.44638 LUMO: 2.26943 factor:1 | 1 (-0.73993) | -1 | -1 |
| G: -6257.17264 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.01139 HOMO: -5.88038 LUMO: 1.90480 factor:1 | 1 (-1.47306) | -1 | -1 |
| G: -6257.17264 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.79931 HOMO: -6.22052 LUMO: 2.17691 factor:1 | 1 (-1.26098) | -1 | -1 |
| G: -6257.17264 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.12465 HOMO: -6.04637 LUMO: 2.23950 factor:1 | 1 (-1.58631) | -1 | -1 |
| G: -6257.17264 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.29190 HOMO: -6.44366 LUMO: 2.24766 factor:1 | 1 (-0.75356) | -1 | -1 |
| G: -6257.17264 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.54137 HOMO: -6.81917 LUMO: 2.08439 factor:1 | 1 (-1.00304) | -1 | -1 |
| G: -6257.17264 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.70067 HOMO: -6.48447 LUMO: 2.28576 factor:1 | 1 (-1.16233) | -1 | -1 |
| G: -6257.17264 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.72303 HOMO: -6.54434 LUMO: 1.99187 factor:1 | 1 (-1.18470) | -1 | -1 |
| G: -6257.17264 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.23194 HOMO: -6.17698 LUMO: -0.65852 factor:1 | 1 (-1.69361) | -1 | -1 |
| G: -6257.17264 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.61699 HOMO: -6.08174 LUMO: -0.58504 factor:1 | 1 (-1.07866) | -1 | -1 |
| G: -6257.17264 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.10606 HOMO: -6.55250 LUMO: -0.86804 factor:1 | 1 (-1.56773) | -1 | -1 |
| G: -6257.17264 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.22174 HOMO: -6.57699 LUMO: -0.89525 factor:1 | 1 (-1.68341) | -1 | -1 |
| G: -6257.17264 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.65519 HOMO: -6.63141 LUMO: -1.04220 factor:1 | 1 (-1.11686) | -1 | -1 |
| G: -6257.17264 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.65386 HOMO: -6.69128 LUMO: -0.76736 factor:1 | 1 (-1.11553) | -1 | -1 |
| G: -6257.17264 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.74317 HOMO: -6.25318 LUMO: -1.03131 factor:1 | 1 (-1.20484) | -1 | -1 |
| G: -6257.17264 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.26386 HOMO: -6.69944 LUMO: 0.01905 factor:1 | 1 (-1.72553) | -1 | -1 |
| G: -6257.17264 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.22043 HOMO: -6.28583 LUMO: 0.38368 factor:1 | 1 (-1.68210) | -1 | -1 |
| G: -6257.17264 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.33443 HOMO: -6.90081 LUMO: -0.83811 factor:1 | 1 (-0.79610) | -1 | -1 |
| G: -6257.17264 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.48512 HOMO: -6.78380 LUMO: -0.10068 factor:1 | 1 (-0.94679) | -1 | -1 |
| G: -6257.17264 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.54994 HOMO: -6.30488 LUMO: -0.98505 factor:1 | 1 (-1.01161) | -1 | -1 |
| G: -6257.17264 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.24715 HOMO: -6.29671 LUMO: -1.79051 factor:1 | 1 (-1.70882) | -1 | -1 |
| G: -6257.17264 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.07654 HOMO: -6.76747 LUMO: -0.22041 factor:1 | 1 (-1.53821) | -1 | -1 |
| G: -6257.17264 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.92540 HOMO: -6.22597 LUMO: -0.94968 factor:1 | 1 (-1.38707) | -1 | -1 |
| G: -6257.17264 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.67819 HOMO: -6.73482 LUMO: 0.05987 factor:1 | 1 (-1.13986) | -1 | -1 |
| G: -6257.17264 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.02285 HOMO: -6.28855 LUMO: 0.34831 factor:1 | 1 (-1.48452) | -1 | -1 |
| G: -6257.17264 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.11256 HOMO: -6.69400 LUMO: 0.25307 factor:1 | 1 (-1.57423) | -1 | -1 |
| G: -6257.17264 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.64286 HOMO: -6.70216 LUMO: 0.61226 factor:1 | 1 (-2.10453) | -1 | -1 |
| G: -6257.17264 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.62762 HOMO: -6.70216 LUMO: 0.17415 factor:1 | 1 (-2.08929) | -1 | -1 |
| G: -6257.17264 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.05558 HOMO: -6.70761 LUMO: 0.24762 factor:1 | 1 (-1.51725) | -1 | -1 |
| G: -6257.17264 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.07869 HOMO: -6.68856 LUMO: -0.84900 factor:1 | 1 (-1.54035) | -1 | -1 |
| G: -6257.17264 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.52033 HOMO: -6.71033 LUMO: -0.38640 factor:1 | 1 (-1.98200) | -1 | -1 |
| G: -6257.17264 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12524.19005 HOMO: -6.24501 LUMO: -0.09252 factor:1 | 1 (-2.65172) | -1 | -1 |
| G: -6257.17264 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.48707 HOMO: -6.81645 LUMO: -0.07347 factor:1 | 1 (-1.94874) | -1 | -1 |
| G: -6257.17264 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.56308 HOMO: -6.49536 LUMO: 0.09796 factor:1 | 1 (-2.02474) | -1 | -1 |
| G: -6257.17264 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12524.17185 HOMO: -6.71033 LUMO: -0.26395 factor:1 | 1 (-2.63352) | -1 | -1 |
| G: -6257.17264 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12524.04918 HOMO: -6.70489 LUMO: -0.09252 factor:1 | 1 (-2.51085) | -1 | -1 |
| G: -6257.17264 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.55900 HOMO: -6.23685 LUMO: 0.39729 factor:1 | 1 (-1.02067) | -1 | -1 |
| G: -6257.17264 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.13197 HOMO: -6.69400 LUMO: -0.05442 factor:1 | 1 (-1.59363) | -1 | -1 |
| G: -6257.17264 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.10470 HOMO: -6.36202 LUMO: 0.09796 factor:1 | 1 (-1.56637) | -1 | -1 |
| G: -6257.17264 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.06100 HOMO: -6.54978 LUMO: 0.15510 factor:1 | 1 (-1.52267) | -1 | -1 |
| G: -6257.17264 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.50991 HOMO: -6.77836 LUMO: 0.25851 factor:1 | 1 (-0.97158) | -1 | -1 |
| G: -6257.17264 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.07139 HOMO: -5.70623 LUMO: 0.73471 factor:1 | 1 (-1.53306) | -1 | -1 |
| G: -6257.17264 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.54172 HOMO: -5.58378 LUMO: 0.89253 factor:1 | 1 (-1.00339) | -1 | -1 |
| G: -6257.17264 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.04960 HOMO: -5.68718 LUMO: 0.87893 factor:1 | 1 (-1.51127) | -1 | -1 |
| G: -6257.17264 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.86369 HOMO: -5.10486 LUMO: 1.11567 factor:1 | 1 (-1.32536) | -1 | -1 |
| G: -6257.17264 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.11648 HOMO: -4.59328 LUMO: 1.27621 factor:1 | 1 (-1.57815) | -1 | -1 |
| G: -6257.17264 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.45508 HOMO: -4.45450 LUMO: 1.82044 factor:1 | 1 (-0.91675) | -1 | -1 |
| G: -6257.17264 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.08380 HOMO: -4.64226 LUMO: 1.70615 factor:1 | 1 (-1.54547) | -1 | -1 |
| G: -6257.17264 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.02679 HOMO: -5.04227 LUMO: 1.04492 factor:1 | 1 (-1.48846) | -1 | -1 |
| G: -6257.17264 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.92627 HOMO: -4.85723 LUMO: 0.93607 factor:1 | 1 (-1.38794) | -1 | -1 |
| G: -6257.17264 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.47625 HOMO: -4.72934 LUMO: 1.00410 factor:1 | 1 (-0.93792) | -1 | -1 |
| G: -6257.17264 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.35143 HOMO: -4.56335 LUMO: 1.56738 factor:1 | 1 (-0.81310) | -1 | -1 |
| G: -6257.17264 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.21042 HOMO: -5.48854 LUMO: 0.33198 factor:1 | 1 (-1.67209) | -1 | -1 |
| G: -6257.17264 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.57801 HOMO: -4.97424 LUMO: 1.33608 factor:1 | 1 (-2.03968) | -1 | -1 |
| G: -6257.17264 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12524.37974 HOMO: -4.60145 LUMO: 1.74697 factor:1 | 1 (-2.84141) | -1 | -1 |
| G: -6257.17264 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12524.37958 HOMO: -5.60010 LUMO: 0.74831 factor:1 | 1 (-2.84125) | -1 | -1 |
| G: -6257.17264 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12524.38793 HOMO: -5.66541 LUMO: 0.66668 factor:1 | 1 (-2.84960) | -1 | -1 |
| G: -6257.17264 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.06073 HOMO: -6.50080 LUMO: 0.07075 factor:1 | 1 (-1.52240) | -1 | -1 |
| G: -6257.17264 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.99844 HOMO: -5.79603 LUMO: 0.22313 factor:1 | 1 (-1.46011) | -1 | -1 |
| G: -6257.17264 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.65506 HOMO: -4.68036 LUMO: 1.29798 factor:1 | 1 (-1.11673) | -1 | -1 |
| G: -6257.17264 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.44858 HOMO: -4.84363 LUMO: 1.34424 factor:1 | 1 (-0.91025) | -1 | -1 |
| G: -6257.17264 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.17725 HOMO: -4.62321 LUMO: 1.82861 factor:1 | 1 (-0.63892) | -1 | -1 |
| G: -6257.17264 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.06894 HOMO: -5.83684 LUMO: 0.82178 factor:1 | 1 (-1.53061) | -1 | -1 |
| G: -6257.17264 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.99446 HOMO: -5.27629 LUMO: 0.57960 factor:1 | 1 (-2.45613) | -1 | -1 |
| G: -6257.17264 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.04992 HOMO: -5.15928 LUMO: -2.96876 factor:1 | 1 (-1.51159) | -1 | -1 |
| G: -6257.17264 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12524.06962 HOMO: -5.08853 LUMO: 0.89253 factor:1 | 1 (-2.53128) | -1 | -1 |
| G: -6257.17264 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.98480 HOMO: -6.42461 LUMO: 0.04354 factor:1 | 1 (-2.44647) | -1 | -1 |
| G: -6257.17264 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.42789 HOMO: -6.42733 LUMO: -0.00544 factor:1 | 1 (-1.88956) | -1 | -1 |
| G: -6257.17264 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.68814 HOMO: -5.87494 LUMO: 0.69933 factor:1 | 1 (-2.14981) | -1 | -1 |
| G: -6257.17264 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.34713 HOMO: -5.07492 LUMO: 1.02587 factor:1 | 1 (-1.80880) | -1 | -1 |
| G: -6257.17264 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.42472 HOMO: -4.44362 LUMO: 1.99187 factor:1 | -1 (0.11361) | -1 | -1 |
| G: -6257.17264 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.03771 HOMO: -5.82052 LUMO: 0.43810 factor:1 | 1 (-1.49937) | -1 | -1 |
| G: -6257.17264 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.13088 HOMO: -5.75793 LUMO: 0.76464 factor:1 | 1 (-1.59255) | -1 | -1 |
| G: -6257.17264 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.81523 HOMO: -5.09669 LUMO: 0.72382 factor:1 | 1 (-1.27689) | -1 | -1 |
| G: -6257.17264 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.32801 HOMO: -6.75387 LUMO: -2.02453 factor:1 | -1 (0.21032) | -1 | -1 |
| G: -6257.17264 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.29926 HOMO: -5.02322 LUMO: 1.14832 factor:1 | 1 (-1.76093) | -1 | -1 |
| G: -6257.17264 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.39894 HOMO: -5.75521 LUMO: 0.73471 factor:1 | 1 (-1.86061) | -1 | -1 |
| G: -6257.17264 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.07025 HOMO: -5.89943 LUMO: 0.54967 factor:1 | 1 (-1.53192) | -1 | -1 |
| G: -6257.17264 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.94582 HOMO: -5.80147 LUMO: 0.72382 factor:1 | 1 (-0.40749) | -1 | -1 |
| G: -6257.17264 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.06520 HOMO: -6.16066 LUMO: 0.39457 factor:1 | 1 (-0.52687) | -1 | -1 |
| G: -6257.17264 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.74008 HOMO: -5.98650 LUMO: 0.76736 factor:1 | 1 (-0.20175) | -1 | -1 |
| G: -6257.17264 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.30678 HOMO: -4.74839 LUMO: 1.88847 factor:1 | 1 (-0.76845) | -1 | -1 |
| G: -6257.17264 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.67126 HOMO: -5.62459 LUMO: 0.26939 factor:1 | 1 (-0.13293) | -1 | -1 |
| G: -6257.17264 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.35280 HOMO: -4.88172 LUMO: 1.30070 factor:1 | -1 (0.18553) | -1 | -1 |
| G: -6257.17264 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.05504 HOMO: -5.09397 LUMO: 0.98505 factor:1 | 1 (-1.51671) | -1 | -1 |
| G: -6257.17264 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.61053 HOMO: -6.50080 LUMO: -0.28300 factor:1 | 1 (-2.07220) | -1 | -1 |
| G: -6257.17264 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.10748 HOMO: -5.04227 LUMO: 1.49935 factor:1 | 1 (-1.56914) | -1 | -1 |
| G: -6257.17264 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.76423 HOMO: -5.22731 LUMO: 0.88437 factor:1 | 1 (-1.22590) | -1 | -1 |
| G: -6257.17264 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.55330 HOMO: -4.95519 LUMO: 1.25717 factor:1 | 1 (-0.01497) | -1 | -1 |
| G: -6257.17264 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.49230 HOMO: -4.61233 LUMO: 1.27621 factor:1 | 1 (-1.95397) | -1 | -1 |
| G: -6257.17264 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.65282 HOMO: -4.70757 LUMO: 1.63813 factor:1 | 1 (-2.11449) | -1 | -1 |
| G: -6257.17264 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.24244 HOMO: -4.85179 LUMO: 1.11839 factor:1 | 1 (-1.70411) | -1 | -1 |
| G: -6257.17264 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.15268 HOMO: -4.97696 LUMO: 1.00138 factor:1 | 1 (-0.61435) | -1 | -1 |
| G: -6257.17264 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.35293 HOMO: -5.64636 LUMO: 0.81090 factor:1 | 1 (-0.81460) | -1 | -1 |
| G: -6257.17264 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.98397 HOMO: -4.37831 LUMO: 1.90208 factor:1 | 1 (-0.44564) | -1 | -1 |
| G: -6257.17264 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.68306 HOMO: -4.67764 LUMO: 1.54561 factor:1 | 1 (-1.14473) | -1 | -1 |
| G: -6257.17264 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.25768 HOMO: -5.87766 LUMO: 0.42994 factor:1 | 1 (-1.71935) | -1 | -1 |
| G: -6257.17264 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.45499 HOMO: -6.03821 LUMO: 0.32382 factor:1 | 1 (-1.91666) | -1 | -1 |
| G: -6257.17264 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.08448 HOMO: -5.99739 LUMO: 0.69389 factor:1 | 1 (-1.54615) | -1 | -1 |
| G: -6257.17264 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.16880 HOMO: -6.43821 LUMO: 0.15238 factor:1 | -1 (0.36953) | -1 | -1 |
| G: -6257.17264 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.62416 HOMO: -6.63414 LUMO: -0.07347 factor:1 | 1 (-0.08582) | -1 | -1 |
| G: -6257.17264 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.45003 HOMO: -6.50080 LUMO: 0.10068 factor:1 | -1 (0.08830) | -1 | -1 |
| G: -6257.17264 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.85411 HOMO: -6.49264 LUMO: 0.19592 factor:1 | 1 (-1.31578) | -1 | -1 |
| G: -6257.17264 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.07681 HOMO: -5.83956 LUMO: 0.12517 factor:1 | 1 (-1.53848) | -1 | -1 |
| G: -6257.17264 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.81631 HOMO: -6.50896 LUMO: 0.19048 factor:1 | 1 (-1.27798) | -1 | -1 |
| G: -6257.17264 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.03663 HOMO: -6.56611 LUMO: 0.04898 factor:1 | -1 (0.50170) | -1 | -1 |
| G: -6257.17264 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.19500 HOMO: -6.68040 LUMO: -0.08436 factor:1 | -1 (0.34333) | -1 | -1 |
| G: -6257.17264 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.11238 HOMO: -6.73754 LUMO: -0.08708 factor:1 | 1 (-0.57405) | -1 | -1 |
| G: -6257.17264 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.29979 HOMO: -6.80285 LUMO: -0.10612 factor:1 | 1 (-0.76146) | -1 | -1 |
| G: -6257.17264 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.93028 HOMO: -6.35658 LUMO: 0.02177 factor:1 | 1 (-0.39195) | -1 | -1 |
| G: -6257.17264 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.42235 HOMO: -5.74160 LUMO: 0.14694 factor:1 | 1 (-0.88402) | -1 | -1 |
| G: -6257.17264 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12520.46637 HOMO: -4.78376 LUMO: 0.92791 factor:1 | -1 (1.07197) | -1 | -1 |
| G: -6257.17264 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.05767 HOMO: -5.90215 LUMO: 0.36463 factor:1 | -1 (0.48066) | -1 | -1 |
| G: -6257.17264 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12520.91318 HOMO: -4.99329 LUMO: 0.85988 factor:1 | -1 (0.62515) | -1 | -1 |
| G: -6257.17264 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.23150 HOMO: -4.93887 LUMO: 1.33608 factor:1 | -1 (0.30684) | -1 | -1 |
| G: -6257.17264 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.30673 HOMO: -5.19193 LUMO: 0.50341 factor:1 | 1 (-0.76840) | -1 | -1 |
| G: -6257.17264 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12520.14056 HOMO: -6.64502 LUMO: -1.98643 factor:1 | -1 (1.39777) | -1 | -1 |
| G: -6257.17264 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12520.90485 HOMO: -5.15384 LUMO: 0.94968 factor:1 | -1 (0.63348) | -1 | -1 |
| G: -6257.17264 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.37099 HOMO: -6.31032 LUMO: 0.08436 factor:1 | 1 (-1.83266) | -1 | -1 |
| G: -6257.17264 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.54522 HOMO: -4.88716 LUMO: 0.82995 factor:1 | 1 (-2.00689) | -1 | -1 |
| G: -6257.17264 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.20625 HOMO: -5.57017 LUMO: 0.19320 factor:1 | 1 (-1.66792) | -1 | -1 |
| G: -6257.17264 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.59751 HOMO: -4.92254 LUMO: 0.93879 factor:1 | 1 (-1.05918) | -1 | -1 |
| G: -6257.17264 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.01099 HOMO: -4.77288 LUMO: 1.60003 factor:1 | 1 (-0.47266) | -1 | -1 |
| G: -6257.17264 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.14792 HOMO: -4.97696 LUMO: 0.89798 factor:1 | 1 (-0.60959) | -1 | -1 |
| G: -6257.17264 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.86274 HOMO: -5.00690 LUMO: 1.14288 factor:1 | 1 (-0.32441) | -1 | -1 |
| G: -6257.17264 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.25772 HOMO: -4.88444 LUMO: 1.48574 factor:1 | 1 (-0.71939) | -1 | -1 |
| G: -6257.17264 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.03201 HOMO: -5.03955 LUMO: 1.51023 factor:1 | -1 (0.50632) | -1 | -1 |
| G: -6257.17264 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12520.97563 HOMO: -5.22459 LUMO: 0.99049 factor:1 | -1 (0.56270) | -1 | -1 |
| G: -6257.17264 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.22633 HOMO: -5.29534 LUMO: 0.96056 factor:1 | 1 (-1.68800) | -1 | -1 |
| G: -6257.17264 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.33554 HOMO: -5.35520 LUMO: 0.68301 factor:1 | 1 (-0.79721) | -1 | -1 |
| G: -6257.17264 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.39992 HOMO: -5.27357 LUMO: 1.18642 factor:1 | 1 (-1.86159) | -1 | -1 |
| G: -6257.17264 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.46159 HOMO: -5.79875 LUMO: 0.61770 factor:1 | 1 (-0.92326) | -1 | -1 |
| G: -6257.17264 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.10089 HOMO: -7.64640 LUMO: -2.45175 factor:1 | 1 (-1.56256) | -1 | -1 |
| G: -6257.17264 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.18751 HOMO: -7.46953 LUMO: -1.29798 factor:1 | 1 (-0.64918) | 1 | 1 |
| G: -6257.17264 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.64349 HOMO: -7.95389 LUMO: -0.37280 factor:1 | 1 (-1.10516) | 1 | 1 |
| G: -6257.17264 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.34156 HOMO: -7.23279 LUMO: -1.19186 factor:1 | 1 (-0.80323) | 1 | 1 |
| G: -6257.17264 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.10810 HOMO: -7.14299 LUMO: -1.12927 factor:1 | 1 (-1.56977) | 1 | 1 |
| G: -6257.17264 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.87647 HOMO: -6.93074 LUMO: 0.31565 factor:1 | 1 (-2.33814) | -1 | -1 |
| G: -6257.17264 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.23091 HOMO: -6.63141 LUMO: 0.28028 factor:1 | 1 (-1.69258) | -1 | -1 |
| G: -6257.17264 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.97920 HOMO: -7.10489 LUMO: -1.07213 factor:1 | 1 (-1.44087) | 1 | 1 |
| G: -6257.17264 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.20281 HOMO: -7.00693 LUMO: -0.69389 factor:1 | -1 (0.33552) | -1 | -1 |
| G: -6257.17264 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.03672 HOMO: -8.50356 LUMO: -1.79595 factor:1 | -1 (0.50161) | -1 | -1 |
| G: -6257.17264 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.34833 HOMO: -7.79334 LUMO: -2.33746 factor:1 | 1 (-0.81000) | -1 | -1 |
| G: -6257.17264 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.00824 HOMO: -7.24367 LUMO: -0.85172 factor:1 | 1 (-0.46991) | 1 | 1 |
| G: -6257.17264 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12520.72349 HOMO: -7.94028 LUMO: -0.20136 factor:1 | -1 (0.81484) | 1 | 1 |
| G: -6257.17264 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12520.86183 HOMO: -7.22462 LUMO: 0.84627 factor:1 | -1 (0.67650) | 1 | 1 |
| G: -6257.17264 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.33374 HOMO: -6.54978 LUMO: 0.34831 factor:1 | 1 (-1.79541) | -1 | -1 |
| G: -6257.17264 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.07267 HOMO: -6.86815 LUMO: 0.32109 factor:1 | 1 (-1.53434) | -1 | -1 |
| G: -6257.17264 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.37036 HOMO: -7.17564 LUMO: -1.28438 factor:1 | 1 (-1.83203) | 1 | 1 |
| G: -6257.17264 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.91688 HOMO: -7.03142 LUMO: -1.12655 factor:1 | 1 (-2.37855) | -1 | -1 |
| G: -6257.17264 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.89904 HOMO: -7.39878 LUMO: 0.15783 factor:1 | 1 (-1.36071) | 1 | 1 |
| G: -6257.17264 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.13499 HOMO: -7.25728 LUMO: 0.42178 factor:1 | 1 (-1.59666) | 1 | 1 |
| G: -6257.17264 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.73158 HOMO: -6.86543 LUMO: 0.93879 factor:1 | 1 (-1.19325) | -1 | -1 |
| G: -6257.17264 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.10204 HOMO: -7.09673 LUMO: -0.69661 factor:1 | 1 (-0.56371) | 1 | 1 |
| G: -6257.17264 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.88212 HOMO: -7.74708 LUMO: 0.01088 factor:1 | 1 (-0.34379) | 1 | 1 |
| G: -6257.17264 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.93741 HOMO: -6.80557 LUMO: 0.46531 factor:1 | 1 (-0.39908) | -1 | -1 |
| G: -6257.17264 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.20558 HOMO: -7.29265 LUMO: 1.31975 factor:1 | 1 (-0.66725) | 1 | 1 |
| G: -6257.17264 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.03282 HOMO: -6.93618 LUMO: 0.29388 factor:1 | 1 (-0.49449) | -1 | -1 |
| G: -6257.17264 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.77001 HOMO: -6.53073 LUMO: 0.71022 factor:1 | 1 (-0.23168) | -1 | -1 |
| G: -6257.17264 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.80114 HOMO: -6.41917 LUMO: -1.24084 factor:1 | 1 (-0.26281) | -1 | -1 |
| G: -6257.17264 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.12433 HOMO: -6.67495 LUMO: -1.09118 factor:1 | 1 (-0.58600) | -1 | -1 |
| G: -6257.17264 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.78881 HOMO: -6.97156 LUMO: -0.53606 factor:1 | 1 (-0.25048) | -1 | -1 |
| G: -6257.17264 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.69504 HOMO: -6.85183 LUMO: -0.45715 factor:1 | 1 (-0.15671) | -1 | -1 |
| G: -6257.17264 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.02789 HOMO: -7.12666 LUMO: -0.67484 factor:1 | 1 (-0.48956) | 1 | 1 |
| G: -6257.17264 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.90601 HOMO: -7.49946 LUMO: -0.14694 factor:1 | 1 (-0.36768) | 1 | 1 |
| G: -6257.17264 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.38239 HOMO: -7.44231 LUMO: 0.58232 factor:1 | 1 (-1.84406) | 1 | 1 |
| G: -6257.17264 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12524.12173 HOMO: -7.36340 LUMO: -0.68301 factor:1 | 1 (-2.58339) | 1 | 1 |
| G: -6257.17264 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.18598 HOMO: -6.13073 LUMO: -0.54967 factor:1 | 1 (-1.64765) | -1 | -1 |
| G: -6257.17264 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.87199 HOMO: -7.81511 LUMO: -0.06531 factor:1 | 1 (-1.33366) | 1 | 1 |
| G: -6257.17264 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.68464 HOMO: -7.26816 LUMO: -1.02587 factor:1 | 1 (-1.14631) | 1 | 1 |
| G: -6257.17264 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12520.91944 HOMO: -7.98110 LUMO: -0.17960 factor:1 | -1 (0.61890) | 1 | 1 |
| G: -6257.17264 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.10888 HOMO: -7.44776 LUMO: -1.00954 factor:1 | -1 (0.42945) | 1 | 1 |
| G: -6257.17264 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.05801 HOMO: -7.47769 LUMO: -1.02859 factor:1 | 1 (-1.51967) | 1 | 1 |
| G: -6257.17264 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.84554 HOMO: -6.75659 LUMO: 0.39457 factor:1 | 1 (-1.30721) | -1 | -1 |
| G: -6257.17264 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12520.99451 HOMO: -6.71849 LUMO: 0.36735 factor:1 | -1 (0.54382) | -1 | -1 |
| G: -6257.17264 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.11854 HOMO: -7.64096 LUMO: -1.43948 factor:1 | -1 (0.41979) | 1 | 1 |
| G: -6257.17264 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12520.96888 HOMO: -7.83144 LUMO: -1.36601 factor:1 | -1 (0.56945) | 1 | 1 |
| G: -6257.17264 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.80683 HOMO: -7.19469 LUMO: 0.35103 factor:1 | 1 (-0.26849) | 1 | 1 |
| G: -6257.17264 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.96079 HOMO: -7.03414 LUMO: 0.20409 factor:1 | 1 (-0.42246) | -1 | -1 |
| G: -6257.17264 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.85243 HOMO: -7.22734 LUMO: 0.31293 factor:1 | 1 (-0.31410) | 1 | 1 |
| G: -6257.17264 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.40030 HOMO: -6.93618 LUMO: 0.56055 factor:1 | 1 (-1.86197) | -1 | -1 |
| G: -6257.17264 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.88844 HOMO: -6.94707 LUMO: -0.88709 factor:1 | 1 (-2.35011) | -1 | -1 |
| G: -6257.17264 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.04258 HOMO: -6.86543 LUMO: -0.83267 factor:1 | 1 (-1.50425) | -1 | -1 |
| G: -6257.17264 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.63416 HOMO: -6.82189 LUMO: -1.15376 factor:1 | 1 (-1.09583) | -1 | -1 |
| G: -6257.17264 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.79069 HOMO: -6.65046 LUMO: -0.46531 factor:1 | 1 (-0.25236) | -1 | -1 |
| G: -6257.17264 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.05736 HOMO: -6.52529 LUMO: 0.20953 factor:1 | 1 (-0.51903) | -1 | -1 |
| G: -6257.17264 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.71506 HOMO: -6.80557 LUMO: 0.44355 factor:1 | 1 (-1.17673) | -1 | -1 |
| G: -6257.17264 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.66134 HOMO: -6.93074 LUMO: -0.81634 factor:1 | 1 (-2.12301) | -1 | -1 |
| G: -6257.17264 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.74877 HOMO: -7.43143 LUMO: -0.45987 factor:1 | 1 (-1.21044) | 1 | 1 |
| G: -6257.17264 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.00562 HOMO: -7.07224 LUMO: -0.68028 factor:1 | 1 (-1.46729) | 1 | 1 |
| G: -6257.17264 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.54778 HOMO: -6.68040 LUMO: -0.71566 factor:1 | 1 (-2.00945) | -1 | -1 |
| G: -6257.17264 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.83193 HOMO: -6.26406 LUMO: -1.09934 factor:1 | 1 (-1.29360) | -1 | -1 |
| G: -6257.17264 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.79152 HOMO: -5.94569 LUMO: -0.72110 factor:1 | 1 (-1.25319) | -1 | -1 |
| G: -6257.17264 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.97218 HOMO: -6.12256 LUMO: -0.42178 factor:1 | 1 (-1.43385) | -1 | -1 |
| G: -6257.17264 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.19140 HOMO: -6.09807 LUMO: 0.11429 factor:1 | 1 (-0.65307) | -1 | -1 |
| G: -6257.17264 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.35192 HOMO: -7.35252 LUMO: -0.55783 factor:1 | 1 (-0.81359) | 1 | 1 |
| G: -6257.17264 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.27606 HOMO: -7.57837 LUMO: -0.76736 factor:1 | 1 (-0.73773) | 1 | 1 |
| G: -6257.17264 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.96805 HOMO: -6.16066 LUMO: 0.01905 factor:1 | 1 (-0.42972) | -1 | -1 |
| G: -6257.17264 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.63879 HOMO: -6.13345 LUMO: -0.41906 factor:1 | 1 (-1.10046) | -1 | -1 |
| G: -6257.17264 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.73667 HOMO: -6.10351 LUMO: -0.33742 factor:1 | 1 (-1.19834) | -1 | -1 |
| G: -6257.17264 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.50237 HOMO: -7.24639 LUMO: -0.51702 factor:1 | 1 (-1.96404) | 1 | 1 |
| G: -6257.17264 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.52520 HOMO: -6.98244 LUMO: -1.82044 factor:1 | 1 (-1.98687) | -1 | -1 |
| G: -6257.17264 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.68986 HOMO: -6.37563 LUMO: -1.67622 factor:1 | 1 (-1.15153) | -1 | -1 |
| G: -6257.17264 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.24946 HOMO: -5.79058 LUMO: -2.55243 factor:1 | 1 (-1.71113) | -1 | -1 |
| G: -6257.17264 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.43285 HOMO: -6.34025 LUMO: -0.27483 factor:1 | 1 (-0.89452) | -1 | -1 |
| G: -6257.17264 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.22722 HOMO: -6.05453 LUMO: -0.51157 factor:1 | -1 (0.31111) | -1 | -1 |
| G: -6257.17264 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.32290 HOMO: -7.53755 LUMO: -0.38912 factor:1 | -1 (0.21543) | 1 | 1 |
| G: -6257.17264 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12520.74735 HOMO: -7.00421 LUMO: -0.50885 factor:1 | -1 (0.79098) | -1 | -1 |
| G: -6257.17264 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12520.95089 HOMO: -7.52123 LUMO: -0.37552 factor:1 | -1 (0.58744) | 1 | 1 |
| G: -6257.17264 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12520.15899 HOMO: -6.70489 LUMO: -1.04764 factor:1 | -1 (1.37935) | -1 | -1 |
| G: -6257.17264 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12520.46275 HOMO: -7.06408 LUMO: -1.16737 factor:1 | -1 (1.07558) | 1 | 1 |
| G: -6257.17264 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12520.58041 HOMO: -6.71849 LUMO: -1.02315 factor:1 | -1 (0.95792) | -1 | -1 |
| G: -6257.17264 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12519.95817 HOMO: -6.16610 LUMO: -0.50885 factor:1 | -1 (1.58017) | -1 | -1 |
| G: -6257.17264 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12520.76474 HOMO: -6.48447 LUMO: 0.07619 factor:1 | -1 (0.77359) | -1 | -1 |
| G: -6257.17264 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.69033 HOMO: -7.06135 LUMO: 0.09796 factor:1 | 1 (-0.15200) | 1 | 1 |
| G: -6257.17264 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.52715 HOMO: -6.47359 LUMO: 0.22585 factor:1 | -1 (0.01118) | -1 | -1 |
| G: -6257.17264 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.22268 HOMO: -6.10896 LUMO: -0.62314 factor:1 | -1 (0.31565) | -1 | -1 |
| G: -6257.17264 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.25642 HOMO: -6.88176 LUMO: -0.96600 factor:1 | -1 (0.28191) | -1 | -1 |
| G: -6257.17264 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.36867 HOMO: -6.67495 LUMO: 0.21769 factor:1 | -1 (0.16966) | -1 | -1 |
| G: -6257.17264 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.06727 HOMO: -6.84911 LUMO: 0.38368 factor:1 | -1 (0.47106) | -1 | -1 |
| G: -6257.17264 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.41313 HOMO: -6.83550 LUMO: 1.29798 factor:1 | -1 (0.12520) | -1 | -1 |
| G: -6257.17264 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12520.91459 HOMO: -6.67495 LUMO: 1.46941 factor:1 | -1 (0.62374) | -1 | -1 |
| G: -6257.17264 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.12621 HOMO: -6.81917 LUMO: 1.30887 factor:1 | -1 (0.41212) | -1 | -1 |
| G: -6257.17264 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.24186 HOMO: -6.56611 LUMO: 0.66396 factor:1 | -1 (0.29647) | -1 | -1 |
| G: -6257.17264 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.04869 HOMO: -6.76203 LUMO: 0.60137 factor:1 | -1 (0.48964) | -1 | -1 |
| G: -6257.17264 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12520.78368 HOMO: -6.55794 LUMO: 0.34286 factor:1 | -1 (0.75465) | -1 | -1 |
| G: -6257.17264 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.34143 HOMO: -6.83550 LUMO: 0.35919 factor:1 | -1 (0.19690) | -1 | -1 |
| G: -6257.17264 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.65409 HOMO: -7.17836 LUMO: 0.63130 factor:1 | 1 (-0.11576) | 1 | 1 |
| G: -6257.17264 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.75327 HOMO: -6.29944 LUMO: -0.69389 factor:1 | 1 (-0.21494) | -1 | -1 |
| G: -6257.17264 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.39299 HOMO: -7.06680 LUMO: -0.95784 factor:1 | -1 (0.14534) | 1 | 1 |
| G: -6257.17264 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.78699 HOMO: -6.84638 LUMO: -0.87076 factor:1 | 1 (-0.24866) | -1 | -1 |
| G: -6257.17264 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.91513 HOMO: -6.96339 LUMO: -1.05308 factor:1 | 1 (-0.37680) | -1 | -1 |
| G: -6257.17264 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.48183 HOMO: -6.75387 LUMO: -1.04220 factor:1 | 1 (-0.94350) | -1 | -1 |
| G: -6257.17264 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.57239 HOMO: -6.71849 LUMO: -0.84355 factor:1 | 1 (-1.03406) | -1 | -1 |
| G: -6257.17264 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.75835 HOMO: -7.16748 LUMO: 0.51702 factor:1 | 1 (-1.22002) | 1 | 1 |
| G: -6257.17264 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.58996 HOMO: -6.92530 LUMO: 0.71566 factor:1 | 1 (-2.05163) | -1 | -1 |
| G: -6257.17264 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.53565 HOMO: -7.11034 LUMO: 0.01905 factor:1 | 1 (-1.99732) | 1 | -1 |
| G: -6257.17264 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.69680 HOMO: -6.79468 LUMO: 0.77008 factor:1 | 1 (-1.15847) | -1 | -1 |
| G: -6257.17264 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.41922 HOMO: -6.52801 LUMO: 0.98233 factor:1 | 1 (-0.88089) | -1 | -1 |
| G: -6257.17264 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.53179 HOMO: -6.76475 LUMO: 0.53334 factor:1 | 1 (-0.99346) | -1 | -1 |
| G: -6257.17264 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.75865 HOMO: -5.29261 LUMO: 0.57416 factor:1 | 1 (-1.22032) | -1 | -1 |
| G: -6257.17264 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.73710 HOMO: -6.57971 LUMO: 0.12789 factor:1 | 1 (-1.19877) | -1 | -1 |
| G: -6257.17264 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.61745 HOMO: -6.99333 LUMO: 0.51430 factor:1 | 1 (-1.07912) | -1 | -1 |
| G: -6257.17264 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.30879 HOMO: -6.41917 LUMO: 0.19048 factor:1 | 1 (-0.77046) | -1 | -1 |
| G: -6257.17264 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.53174 HOMO: -6.16066 LUMO: 1.77146 factor:1 | 1 (-0.99341) | -1 | -1 |
| G: -6257.17264 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.37905 HOMO: -6.90353 LUMO: 1.65717 factor:1 | 1 (-0.84072) | -1 | -1 |
| G: -6257.17264 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.42733 HOMO: -5.94569 LUMO: 1.29526 factor:1 | 1 (-0.88900) | -1 | -1 |
| G: -6257.17264 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.31301 HOMO: -6.60420 LUMO: 1.33880 factor:1 | 1 (-0.77468) | -1 | -1 |
| G: -6257.17264 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.30907 HOMO: -6.23957 LUMO: 0.09524 factor:1 | 1 (-0.77074) | -1 | -1 |
| G: -6257.17264 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.40817 HOMO: -6.80013 LUMO: 1.34696 factor:1 | 1 (-0.86984) | -1 | -1 |
| G: -6257.17264 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.54755 HOMO: -7.53483 LUMO: -1.52384 factor:1 | 1 (-1.00922) | -1 | -1 |
| G: -6257.17264 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.20281 HOMO: -7.62463 LUMO: -1.65717 factor:1 | 1 (-0.66447) | -1 | -1 |
| G: -6257.17264 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.34948 HOMO: -7.62463 LUMO: -1.61364 factor:1 | -1 (0.18885) | -1 | -1 |
| G: -6257.17264 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.12768 HOMO: -8.04096 LUMO: -1.66806 factor:1 | -1 (0.41065) | -1 | -1 |
| G: -6257.17264 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.12474 HOMO: -7.18381 LUMO: -1.17553 factor:1 | -1 (0.41359) | 1 | 1 |
| G: -6257.17264 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.83395 HOMO: -7.69538 LUMO: -1.36601 factor:1 | 1 (-1.29562) | 1 | 1 |
| G: -6257.17264 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.58820 HOMO: -7.95117 LUMO: -1.48302 factor:1 | 1 (-1.04987) | -1 | -1 |
| G: -6257.17264 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.28184 HOMO: -6.98516 LUMO: 0.35919 factor:1 | -1 (0.25649) | -1 | -1 |
| G: -6257.17264 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.26004 HOMO: -7.91579 LUMO: -0.32109 factor:1 | -1 (0.27829) | 1 | 1 |
| G: -6257.17264 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.68183 HOMO: -6.75659 LUMO: -0.03537 factor:1 | 1 (-1.14350) | -1 | -1 |
| G: -6257.17264 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.30994 HOMO: -7.78518 LUMO: -2.36467 factor:1 | 1 (-0.77161) | -1 | -1 |
| G: -6257.17264 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.76053 HOMO: -7.96477 LUMO: -2.75651 factor:1 | 1 (-1.22220) | -1 | -1 |
| G: -6257.17264 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.42861 HOMO: -7.60286 LUMO: -2.35106 factor:1 | 1 (-0.89027) | -1 | -1 |
| G: -6257.17264 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.18885 HOMO: -7.38245 LUMO: -1.21635 factor:1 | 1 (-0.65052) | 1 | 1 |
| G: -6257.17264 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.50170 HOMO: -7.91579 LUMO: -1.50479 factor:1 | -1 (0.03663) | -1 | -1 |
| G: -6257.17264 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.36208 HOMO: -8.07362 LUMO: -0.28028 factor:1 | -1 (0.17625) | 1 | 1 |
| G: -6257.17264 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.47719 HOMO: -7.38245 LUMO: -1.15921 factor:1 | -1 (0.06114) | 1 | 1 |
| G: -6257.17264 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.14836 HOMO: -7.18653 LUMO: -0.94968 factor:1 | -1 (0.38997) | 1 | 1 |
| G: -6257.17264 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.27950 HOMO: -6.88448 LUMO: 0.38096 factor:1 | -1 (0.25883) | -1 | -1 |
| G: -6257.17264 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.20603 HOMO: -6.97972 LUMO: 0.43266 factor:1 | -1 (0.33231) | -1 | -1 |
| G: -6257.17264 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.41621 HOMO: -6.88992 LUMO: -0.43538 factor:1 | -1 (0.12212) | -1 | -1 |
| G: -6257.17264 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.47961 HOMO: -7.97021 LUMO: -0.17143 factor:1 | -1 (0.05872) | 1 | 1 |
| G: -6257.17264 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.72666 HOMO: -6.92530 LUMO: 0.77280 factor:1 | 1 (-0.18833) | -1 | -1 |
| G: -6257.17264 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.01263 HOMO: -7.89674 LUMO: -0.09796 factor:1 | 1 (-0.47429) | 1 | 1 |
| G: -6257.17264 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.25663 HOMO: -7.02870 LUMO: 0.88709 factor:1 | 1 (-0.71830) | -1 | -1 |
| G: -6257.17264 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.33117 HOMO: -6.78380 LUMO: 0.22041 factor:1 | -1 (0.20716) | -1 | -1 |
| G: -6257.17264 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.39381 HOMO: -7.24911 LUMO: -0.82178 factor:1 | -1 (0.14452) | 1 | 1 |
| G: -6257.17264 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.25571 HOMO: -6.77019 LUMO: 0.52790 factor:1 | -1 (0.28262) | -1 | -1 |
| G: -6257.17264 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.52382 HOMO: -8.56070 LUMO: -1.83405 factor:1 | 1 (-0.98549) | -1 | -1 |
| G: -6257.17264 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.25768 HOMO: -7.74164 LUMO: -2.36195 factor:1 | 1 (-1.71935) | -1 | -1 |
| G: -6257.17264 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12524.11313 HOMO: -7.39878 LUMO: -2.41637 factor:1 | 1 (-2.57480) | -1 | -1 |
| G: -6257.17264 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.87350 HOMO: -7.61647 LUMO: -2.34018 factor:1 | 1 (-2.33517) | -1 | -1 |
| G: -6257.17264 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12524.45047 HOMO: -6.93346 LUMO: -0.57688 factor:1 | 1 (-2.91214) | -1 | -1 |
| G: -6257.17264 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12524.17819 HOMO: -6.85183 LUMO: -1.00410 factor:1 | 1 (-2.63986) | -1 | -1 |
| G: -6257.17264 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.99620 HOMO: -7.18925 LUMO: -1.12655 factor:1 | 1 (-2.45787) | 1 | 1 |
| G: -6257.17264 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.30568 HOMO: -6.85183 LUMO: -1.60275 factor:1 | 1 (-1.76735) | -1 | -1 |
| G: -6257.17264 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12524.13141 HOMO: -7.51578 LUMO: 0.12517 factor:1 | 1 (-2.59308) | 1 | 1 |
| G: -6257.17264 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.64781 HOMO: -7.36068 LUMO: 0.05714 factor:1 | 1 (-2.10948) | 1 | 1 |
| G: -6257.17264 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.39929 HOMO: -7.49674 LUMO: 0.18776 factor:1 | 1 (-1.86096) | 1 | 1 |
| G: -6257.17264 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.36211 HOMO: -7.09401 LUMO: -1.24900 factor:1 | -1 (0.17622) | 1 | 1 |
| G: -6257.17264 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.34856 HOMO: -7.22462 LUMO: -1.61364 factor:1 | -1 (0.18977) | -1 | -1 |
| G: -6257.17264 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.33479 HOMO: -7.74436 LUMO: -0.18776 factor:1 | -1 (0.20354) | 1 | 1 |
| G: -6257.17264 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.99083 HOMO: -7.35252 LUMO: 0.75376 factor:1 | 1 (-0.45250) | 1 | 1 |
| G: -6257.17264 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.26240 HOMO: -7.75252 LUMO: 0.00816 factor:1 | 1 (-0.72407) | 1 | 1 |
| G: -6257.17264 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.24847 HOMO: -7.06680 LUMO: 0.24490 factor:1 | 1 (-0.71014) | 1 | 1 |
| G: -6257.17264 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.85934 HOMO: -7.49129 LUMO: 0.14150 factor:1 | 1 (-0.32101) | 1 | 1 |
| G: -6257.17264 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.36980 HOMO: -6.90625 LUMO: -1.11295 factor:1 | 1 (-0.83147) | -1 | -1 |
| G: -6257.17264 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.06710 HOMO: -6.78380 LUMO: -0.93063 factor:1 | 1 (-0.52877) | -1 | -1 |
| G: -6257.17264 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.91749 HOMO: -7.79878 LUMO: 0.30477 factor:1 | 1 (-0.37916) | 1 | 1 |
| G: -6257.17264 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.22931 HOMO: -7.87498 LUMO: 0.61770 factor:1 | 1 (-0.69098) | 1 | 1 |
| G: -6257.17264 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.85964 HOMO: -7.23823 LUMO: 0.30205 factor:1 | 1 (-0.32131) | 1 | 1 |
| G: -6257.17264 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.96638 HOMO: -7.67633 LUMO: 0.13061 factor:1 | 1 (-2.42804) | 1 | 1 |
| G: -6257.17264 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.06084 HOMO: -7.79606 LUMO: 0.34558 factor:1 | 1 (-1.52250) | 1 | 1 |
| G: -6257.17264 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.24315 HOMO: -6.66135 LUMO: -2.60141 factor:1 | 1 (-1.70482) | -1 | -1 |
| G: -6257.17264 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.99555 HOMO: -7.03142 LUMO: 0.50885 factor:1 | 1 (-2.45722) | -1 | -1 |
| G: -6257.17264 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.99911 HOMO: -7.05591 LUMO: -0.06531 factor:1 | 1 (-2.46078) | -1 | -1 |
| G: -6257.17264 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.12503 HOMO: -7.45592 LUMO: -1.39594 factor:1 | 1 (-1.58670) | 1 | 1 |
| G: -6257.17264 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.64798 HOMO: -7.22462 LUMO: -1.10478 factor:1 | 1 (-2.10964) | 1 | 1 |
| G: -6257.17264 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.72741 HOMO: -8.14709 LUMO: -0.55783 factor:1 | 1 (-1.18908) | 1 | 1 |
| G: -6257.17264 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.18712 HOMO: -7.22190 LUMO: -1.14560 factor:1 | 1 (-1.64879) | 1 | 1 |
| G: -6257.17264 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.38773 HOMO: -7.28721 LUMO: -1.14016 factor:1 | 1 (-1.84939) | 1 | 1 |
| G: -6257.17264 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.44825 HOMO: -6.97156 LUMO: 0.51702 factor:1 | 1 (-0.90992) | -1 | -1 |
| G: -6257.17264 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.33481 HOMO: -7.37156 LUMO: 0.29388 factor:1 | 1 (-0.79648) | 1 | -1 |
| G: -6257.17264 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.30591 HOMO: -7.66273 LUMO: -1.59731 factor:1 | 1 (-0.76758) | -1 | -1 |
| G: -6257.17264 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.01121 HOMO: -7.50490 LUMO: -1.49935 factor:1 | 1 (-0.47288) | -1 | -1 |
| G: -6257.17264 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.52251 HOMO: -7.61102 LUMO: -1.45581 factor:1 | 1 (-0.98418) | 1 | 1 |
| G: -6257.17264 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.10285 HOMO: -7.58653 LUMO: -1.61091 factor:1 | 1 (-1.56452) | -1 | -1 |
| G: -6257.17264 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.32762 HOMO: -7.36068 LUMO: -1.14560 factor:1 | 1 (-0.78929) | 1 | 1 |
| G: -6257.17264 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.10093 HOMO: -6.96339 LUMO: 0.26939 factor:1 | 1 (-0.56260) | -1 | -1 |
| G: -6257.17264 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.33230 HOMO: -6.53617 LUMO: 0.22313 factor:1 | 1 (-0.79397) | -1 | -1 |
| G: -6257.17264 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12519.99125 HOMO: -7.33619 LUMO: -1.02587 factor:1 | -1 (1.54708) | 1 | 1 |
| G: -6257.17264 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12519.98821 HOMO: -6.87904 LUMO: 0.33742 factor:1 | -1 (1.55012) | -1 | -1 |
| G: -6257.17264 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12520.57839 HOMO: -6.88448 LUMO: 0.58777 factor:1 | -1 (0.95994) | -1 | -1 |
| G: -6257.17264 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12520.86689 HOMO: -6.55522 LUMO: -1.51295 factor:1 | -1 (0.67144) | -1 | -1 |
| G: -6257.17264 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.54065 HOMO: -7.43415 LUMO: 0.10612 factor:1 | 1 (-2.00232) | 1 | 1 |
| G: -6257.17264 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.35647 HOMO: -7.54300 LUMO: -0.02449 factor:1 | 1 (-0.81814) | 1 | 1 |
| G: -6257.17264 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.57089 HOMO: -7.42054 LUMO: 0.28028 factor:1 | 1 (-1.03256) | 1 | 1 |
| G: -6257.17264 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.16808 HOMO: -6.98244 LUMO: -0.95784 factor:1 | 1 (-0.62975) | -1 | -1 |
| G: -6257.17264 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.00014 HOMO: -6.96884 LUMO: -1.12383 factor:1 | 1 (-0.46180) | -1 | -1 |
| G: -6257.17264 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.19393 HOMO: -6.80829 LUMO: -0.98233 factor:1 | 1 (-0.65560) | -1 | -1 |
| G: -6257.17264 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12520.87835 HOMO: -7.60830 LUMO: 0.58504 factor:1 | -1 (0.65998) | 1 | 1 |
| G: -6257.17264 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.04390 HOMO: -7.52123 LUMO: 0.08163 factor:1 | -1 (0.49443) | 1 | 1 |
| G: -6257.17264 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.00278 HOMO: -7.59742 LUMO: 0.00272 factor:1 | -1 (0.53555) | 1 | 1 |
| G: -6257.17264 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.29219 HOMO: -6.99333 LUMO: -1.33880 factor:1 | 1 (-1.75386) | -1 | -1 |
| G: -6257.17264 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.53242 HOMO: -6.63958 LUMO: -1.39322 factor:1 | 1 (-0.99409) | -1 | -1 |
| G: -6257.17264 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.03509 HOMO: -7.86137 LUMO: 0.01633 factor:1 | 1 (-1.49676) | 1 | 1 |
| G: -6257.17264 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.22090 HOMO: -7.29537 LUMO: 0.14694 factor:1 | 1 (-0.68257) | 1 | 1 |
| G: -6257.17264 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.56942 HOMO: -6.95523 LUMO: 0.48708 factor:1 | 1 (-1.03109) | -1 | -1 |
| G: -6257.17264 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.32022 HOMO: -7.10217 LUMO: -1.10478 factor:1 | 1 (-0.78189) | 1 | 1 |
| G: -6257.17264 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.33835 HOMO: -6.88176 LUMO: -0.96328 factor:1 | 1 (-0.80001) | -1 | -1 |
| G: -6257.17264 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.32847 HOMO: -7.89130 LUMO: -0.13334 factor:1 | 1 (-0.79014) | 1 | 1 |
| G: -6257.17264 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.46436 HOMO: -7.75252 LUMO: 0.25579 factor:1 | 1 (-0.92603) | 1 | 1 |
| G: -6257.17264 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.13369 HOMO: -6.87632 LUMO: -0.93063 factor:1 | 1 (-0.59536) | -1 | -1 |
| G: -6257.17264 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.11336 HOMO: -6.78108 LUMO: -0.86804 factor:1 | 1 (-0.57503) | -1 | -1 |
| G: -6257.17264 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.26400 HOMO: -5.98106 LUMO: 0.10340 factor:1 | 1 (-0.72567) | -1 | -1 |
| G: -6257.17264 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.01551 HOMO: -6.40284 LUMO: -0.87349 factor:1 | 1 (-0.47718) | -1 | -1 |
| G: -6257.17264 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.14294 HOMO: -6.77019 LUMO: -1.20819 factor:1 | 1 (-0.60461) | -1 | -1 |
| G: -6257.17264 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.33297 HOMO: -6.90081 LUMO: -1.00682 factor:1 | -1 (0.20536) | -1 | -1 |
| G: -6257.17264 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.31362 HOMO: -6.59060 LUMO: -0.26667 factor:1 | -1 (0.22471) | -1 | -1 |
| G: -6257.17264 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.29944 HOMO: -6.50896 LUMO: -0.48708 factor:1 | -1 (0.23889) | -1 | -1 |
| G: -6257.17264 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.28584 HOMO: -6.20420 LUMO: -0.73471 factor:1 | -1 (0.25249) | -1 | -1 |
| G: -6257.17264 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.25239 HOMO: -6.17154 LUMO: -0.68573 factor:1 | -1 (0.28594) | -1 | -1 |
| G: -6257.17264 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.10540 HOMO: -6.21236 LUMO: 0.09796 factor:1 | -1 (0.43293) | -1 | -1 |
| G: -6257.17264 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.61168 HOMO: -6.38379 LUMO: 0.58232 factor:1 | 1 (-1.07335) | -1 | -1 |
| G: -6257.17264 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.60034 HOMO: -7.42871 LUMO: 0.40273 factor:1 | 1 (-1.06201) | 1 | 1 |
| G: -6257.17264 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.24716 HOMO: -6.54978 LUMO: 0.26395 factor:1 | 1 (-0.70883) | -1 | -1 |
| G: -6257.17264 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.29144 HOMO: -7.14027 LUMO: 0.14150 factor:1 | -1 (0.24689) | 1 | 1 |
| G: -6257.17264 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12520.90425 HOMO: -7.25456 LUMO: -0.15783 factor:1 | -1 (0.63408) | 1 | 1 |
| G: -6257.17264 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.09919 HOMO: -6.90897 LUMO: 0.63403 factor:1 | -1 (0.43914) | -1 | -1 |
| G: -6257.17264 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.17898 HOMO: -6.49264 LUMO: 0.71022 factor:1 | -1 (0.35935) | -1 | -1 |
| G: -6257.17264 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.69441 HOMO: -6.56067 LUMO: -1.03947 factor:1 | 1 (-1.15608) | -1 | -1 |
| G: -6257.17264 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.27225 HOMO: -6.79196 LUMO: -1.12655 factor:1 | 1 (-0.73392) | -1 | -1 |
| G: -6257.17264 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.71808 HOMO: -6.95251 LUMO: -1.09118 factor:1 | 1 (-1.17975) | -1 | -1 |
| G: -6257.17264 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.84035 HOMO: -7.47225 LUMO: -0.22041 factor:1 | 1 (-0.30202) | 1 | 1 |
| G: -6257.17264 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.07880 HOMO: -7.13483 LUMO: -0.98505 factor:1 | 1 (-0.54047) | 1 | 1 |
| G: -6257.17264 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.57528 HOMO: -6.99061 LUMO: -1.05852 factor:1 | 1 (-1.03694) | -1 | -1 |
| G: -6257.17264 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.77556 HOMO: -6.52257 LUMO: -1.11022 factor:1 | 1 (-0.23723) | -1 | -1 |
| G: -6257.17264 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.15622 HOMO: -6.75114 LUMO: -1.09934 factor:1 | 1 (-0.61789) | -1 | -1 |
| G: -6257.17264 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.96484 HOMO: -6.82189 LUMO: -0.89253 factor:1 | 1 (-0.42651) | -1 | -1 |
| G: -6257.17264 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.80110 HOMO: -6.83278 LUMO: -0.97961 factor:1 | 1 (-1.26277) | -1 | -1 |
| G: -6257.17264 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.57598 HOMO: -6.65318 LUMO: -0.84355 factor:1 | 1 (-1.03765) | -1 | -1 |
| G: -6257.17264 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.26346 HOMO: -6.75931 LUMO: -0.88437 factor:1 | 1 (-0.72513) | -1 | -1 |
| G: -6257.17264 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.07312 HOMO: -6.19059 LUMO: -0.45715 factor:1 | 1 (-0.53479) | -1 | -1 |
| G: -6257.17264 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12520.70291 HOMO: -7.09673 LUMO: -2.01908 factor:1 | -1 (0.83542) | -1 | -1 |
| G: -6257.17264 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.24352 HOMO: -7.88042 LUMO: 0.38640 factor:1 | -1 (0.29481) | 1 | 1 |
| G: -6257.17264 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12520.90101 HOMO: -7.83144 LUMO: 0.14422 factor:1 | -1 (0.63732) | 1 | 1 |
| G: -6257.17264 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.18964 HOMO: -7.46408 LUMO: 0.44627 factor:1 | 1 (-0.65130) | 1 | 1 |
| G: -6257.17264 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.10776 HOMO: -7.12394 LUMO: -2.04902 factor:1 | 1 (-0.56943) | -1 | -1 |
| G: -6257.17264 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.25282 HOMO: -6.78380 LUMO: -1.11295 factor:1 | 1 (-0.71449) | -1 | -1 |
| G: -6257.17264 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.14299 HOMO: -7.12938 LUMO: -0.23674 factor:1 | 1 (-0.60466) | 1 | 1 |
| G: -6257.17264 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.95924 HOMO: -6.14705 LUMO: -0.20409 factor:1 | 1 (-0.42091) | -1 | -1 |
| G: -6257.17264 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.32969 HOMO: -6.50080 LUMO: -0.28300 factor:1 | 1 (-0.79136) | -1 | -1 |
| G: -6257.17264 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.71090 HOMO: -6.50352 LUMO: -0.62042 factor:1 | 1 (-1.17257) | -1 | -1 |
| G: -6257.17264 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.39152 HOMO: -6.46543 LUMO: -0.53879 factor:1 | 1 (-0.85319) | -1 | -1 |
| G: -6257.17264 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.86285 HOMO: -7.32803 LUMO: -0.52790 factor:1 | 1 (-0.32452) | 1 | 1 |
| G: -6257.17264 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.17864 HOMO: -5.94025 LUMO: -0.17687 factor:1 | 1 (-0.64031) | -1 | -1 |
| G: -6257.17264 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.67092 HOMO: -5.62187 LUMO: 0.05714 factor:1 | 1 (-1.13259) | -1 | -1 |
| G: -6257.17264 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.85631 HOMO: -7.03414 LUMO: -1.04492 factor:1 | 1 (-1.31798) | -1 | -1 |
| G: -6257.17264 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.91014 HOMO: -6.75387 LUMO: -2.02181 factor:1 | 1 (-1.37181) | -1 | -1 |
| G: -6257.17264 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.82777 HOMO: -6.55250 LUMO: -0.75648 factor:1 | 1 (-1.28944) | -1 | -1 |
| G: -6257.17264 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.48360 HOMO: -6.81101 LUMO: -1.02043 factor:1 | 1 (-0.94527) | -1 | -1 |
| G: -6257.17264 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.82774 HOMO: -6.69672 LUMO: -2.81910 factor:1 | 1 (-1.28941) | -1 | -1 |
| G: -6257.17264 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.80586 HOMO: -6.69128 LUMO: -2.58236 factor:1 | 1 (-1.26753) | -1 | -1 |
| G: -6257.17264 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.10880 HOMO: -6.73482 LUMO: -2.06807 factor:1 | -1 (0.42953) | -1 | -1 |
| G: -6257.17264 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.21830 HOMO: -7.66545 LUMO: 0.17143 factor:1 | -1 (0.32003) | 1 | 1 |
| G: -6257.17264 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12520.83448 HOMO: -6.87904 LUMO: -1.25172 factor:1 | -1 (0.70385) | -1 | -1 |
| G: -6257.17264 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.38478 HOMO: -6.84366 LUMO: -0.19320 factor:1 | -1 (0.15355) | -1 | -1 |
| G: -6257.17264 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12520.91688 HOMO: -6.97972 LUMO: -0.97961 factor:1 | -1 (0.62145) | -1 | -1 |
| G: -6257.17264 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12520.75040 HOMO: -6.72121 LUMO: -0.70477 factor:1 | -1 (0.78793) | -1 | -1 |
| G: -6257.17264 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12520.96765 HOMO: -7.18925 LUMO: 0.40001 factor:1 | -1 (0.57068) | 1 | 1 |
| G: -6257.17264 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.78579 HOMO: -6.72121 LUMO: 0.19592 factor:1 | 1 (-0.24746) | -1 | -1 |
| G: -6257.17264 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.16363 HOMO: -6.85999 LUMO: -0.39457 factor:1 | -1 (0.37470) | -1 | -1 |
| G: -6257.17264 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.15362 HOMO: -6.90625 LUMO: 0.05987 factor:1 | -1 (0.38471) | -1 | -1 |
| G: -6257.17264 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.39340 HOMO: -7.00421 LUMO: 0.37552 factor:1 | -1 (0.14493) | -1 | -1 |
| G: -6257.17264 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.84914 HOMO: -6.56883 LUMO: -0.97689 factor:1 | 1 (-0.31081) | -1 | -1 |
| G: -6257.17264 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12520.69807 HOMO: -6.66679 LUMO: 0.56055 factor:1 | -1 (0.84026) | -1 | -1 |
| G: -6257.17264 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.79423 HOMO: -6.75931 LUMO: 0.32926 factor:1 | 1 (-0.25590) | -1 | -1 |
| G: -6257.17264 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.77575 HOMO: -6.53617 LUMO: -1.06397 factor:1 | 1 (-0.23742) | -1 | -1 |
| G: -6257.17264 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.86163 HOMO: -6.78108 LUMO: 0.42722 factor:1 | 1 (-0.32330) | -1 | -1 |
| G: -6257.17264 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12520.57018 HOMO: -7.05319 LUMO: 0.61498 factor:1 | -1 (0.96815) | -1 | -1 |
| G: -6257.17264 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12520.78409 HOMO: -6.78380 LUMO: 1.49391 factor:1 | -1 (0.75425) | -1 | -1 |
| G: -6257.17264 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12520.64659 HOMO: -7.21102 LUMO: 0.27211 factor:1 | -1 (0.89174) | 1 | 1 |
| G: -6257.17264 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12520.78956 HOMO: -6.67223 LUMO: 0.81362 factor:1 | -1 (0.74878) | -1 | -1 |
| G: -6257.17264 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12520.57924 HOMO: -6.69944 LUMO: 1.40683 factor:1 | -1 (0.95909) | -1 | -1 |
| G: -6257.17264 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.48007 HOMO: -7.02598 LUMO: 1.46941 factor:1 | -1 (0.05826) | -1 | -1 |
| G: -6257.17264 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.71986 HOMO: -5.85045 LUMO: -0.76736 factor:1 | 1 (-0.18153) | -1 | -1 |
| G: -6257.17264 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.68832 HOMO: -6.53890 LUMO: -0.50885 factor:1 | 1 (-0.14999) | -1 | -1 |
| G: -6257.17264 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.80963 HOMO: -6.42733 LUMO: -0.63947 factor:1 | 1 (-0.27130) | -1 | -1 |
| G: -6257.17264 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.52282 HOMO: -6.82189 LUMO: -0.85444 factor:1 | -1 (0.01551) | -1 | -1 |
| G: -6257.17264 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.24246 HOMO: -6.97428 LUMO: -1.22179 factor:1 | -1 (0.29587) | -1 | -1 |
| G: -6257.17264 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.13242 HOMO: -6.93346 LUMO: -1.09934 factor:1 | -1 (0.40591) | -1 | -1 |
| G: -6257.17264 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.39071 HOMO: -7.17292 LUMO: -1.11839 factor:1 | -1 (0.14762) | 1 | 1 |
| G: -6257.17264 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.47515 HOMO: -7.00965 LUMO: -1.23268 factor:1 | -1 (0.06318) | -1 | -1 |
| G: -6257.17264 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.13343 HOMO: -6.73210 LUMO: -1.12383 factor:1 | -1 (0.40491) | -1 | -1 |
| G: -6257.17264 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.34649 HOMO: -7.61375 LUMO: -0.11973 factor:1 | -1 (0.19184) | 1 | 1 |
| G: -6257.17264 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.91880 HOMO: -7.42327 LUMO: 0.41906 factor:1 | 1 (-0.38047) | 1 | 1 |
| G: -6257.17264 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.17004 HOMO: -6.94162 LUMO: -1.01771 factor:1 | 1 (-0.63171) | -1 | -1 |
| G: -6257.17264 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.70247 HOMO: -6.82189 LUMO: -0.92791 factor:1 | 1 (-0.16414) | -1 | -1 |
| G: -6257.17264 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.93322 HOMO: -6.92258 LUMO: -1.73881 factor:1 | 1 (-0.39489) | -1 | -1 |
| G: -6257.17264 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.94160 HOMO: -6.50896 LUMO: -1.60819 factor:1 | 1 (-0.40327) | -1 | -1 |
| G: -6257.17264 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12520.76896 HOMO: -6.38379 LUMO: -2.18780 factor:1 | -1 (0.76937) | -1 | -1 |
| G: -6257.17264 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12520.98725 HOMO: -6.48992 LUMO: -0.97417 factor:1 | -1 (0.55108) | -1 | -1 |
| G: -6257.17264 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.36067 HOMO: -6.01644 LUMO: -0.04354 factor:1 | -1 (0.17766) | -1 | -1 |
| G: -6257.17264 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.43354 HOMO: -6.70761 LUMO: -0.14422 factor:1 | -1 (0.10479) | -1 | -1 |
| G: -6257.17264 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.43852 HOMO: -6.70216 LUMO: 0.14422 factor:1 | -1 (0.09981) | -1 | -1 |
| G: -6257.17264 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.38987 HOMO: -7.07224 LUMO: -0.10885 factor:1 | -1 (0.14847) | 1 | 1 |
| G: -6257.17264 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.57327 HOMO: -7.52667 LUMO: -0.74287 factor:1 | 1 (-0.03494) | 1 | 1 |
| G: -6257.17264 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.22633 HOMO: -6.48447 LUMO: -0.96056 factor:1 | -1 (0.31201) | -1 | -1 |
| G: -6257.17264 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.44930 HOMO: -6.22597 LUMO: -0.41361 factor:1 | -1 (0.08904) | -1 | -1 |
| G: -6257.17264 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.13625 HOMO: -6.12256 LUMO: -1.05852 factor:1 | 1 (-0.59792) | -1 | -1 |
| G: -6257.17264 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.87992 HOMO: -6.97428 LUMO: -0.60681 factor:1 | 1 (-0.34158) | -1 | -1 |
| G: -6257.17264 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.27954 HOMO: -6.78380 LUMO: -0.88981 factor:1 | 1 (-0.74121) | -1 | -1 |
| G: -6257.17264 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.04751 HOMO: -6.85999 LUMO: 0.07891 factor:1 | 1 (-0.50918) | -1 | -1 |
| G: -6257.17264 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.37865 HOMO: -7.08312 LUMO: -0.60137 factor:1 | 1 (-0.84031) | 1 | 1 |
| G: -6257.17264 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.40431 HOMO: -6.57699 LUMO: -0.68028 factor:1 | -1 (0.13402) | -1 | -1 |
| G: -6257.17264 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.13532 HOMO: -6.09807 LUMO: -0.31837 factor:1 | 1 (-0.59699) | -1 | -1 |
| G: -6257.17264 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.55790 HOMO: -6.10624 LUMO: 0.14966 factor:1 | 1 (-0.01956) | -1 | -1 |
| G: -6257.17264 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.82321 HOMO: -6.77019 LUMO: -0.95784 factor:1 | 1 (-0.28488) | -1 | -1 |
| G: -6257.17264 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.30137 HOMO: -5.93208 LUMO: -0.44627 factor:1 | 1 (-0.76303) | -1 | -1 |
| G: -6257.17264 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.57545 HOMO: -6.12256 LUMO: -0.27756 factor:1 | 1 (-0.03712) | -1 | -1 |
| G: -6257.17264 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.80040 HOMO: -5.98106 LUMO: -0.37824 factor:1 | 1 (-0.26207) | -1 | -1 |
| G: -6257.17264 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.60731 HOMO: -7.06408 LUMO: -1.12927 factor:1 | 1 (-0.06898) | 1 | 1 |
| G: -6257.17264 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.83167 HOMO: -6.70761 LUMO: -0.98505 factor:1 | 1 (-0.29334) | -1 | -1 |
| G: -6257.17264 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.06465 HOMO: -7.00965 LUMO: -0.42722 factor:1 | 1 (-0.52632) | -1 | -1 |
| G: -6257.17264 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.02860 HOMO: -5.96201 LUMO: -0.59049 factor:1 | 1 (-0.49027) | -1 | -1 |
| G: -6257.17264 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.22449 HOMO: -6.34570 LUMO: -1.68438 factor:1 | 1 (-0.68616) | -1 | -1 |
| G: -6257.17264 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.27791 HOMO: -6.97156 LUMO: -1.85854 factor:1 | 1 (-0.73958) | -1 | -1 |
| G: -6257.17264 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.64649 HOMO: -5.91848 LUMO: -2.51433 factor:1 | 1 (-1.10816) | -1 | -1 |
| G: -6257.17264 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.78986 HOMO: -6.39195 LUMO: -1.66262 factor:1 | 1 (-1.25153) | -1 | -1 |
| G: -6257.17264 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.75827 HOMO: -6.50352 LUMO: 0.19592 factor:1 | 1 (-1.21994) | -1 | -1 |
| G: -6257.17264 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.50164 HOMO: -6.45998 LUMO: 0.34831 factor:1 | 1 (-0.96331) | -1 | -1 |
| G: -6257.17264 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.42621 HOMO: -7.05319 LUMO: 0.23402 factor:1 | 1 (-0.88788) | -1 | -1 |
| G: -6257.17264 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.12842 HOMO: -6.61237 LUMO: 0.18232 factor:1 | -1 (0.40991) | -1 | -1 |
| G: -6257.17264 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.13451 HOMO: -6.57427 LUMO: 0.40545 factor:1 | -1 (0.40382) | -1 | -1 |
| G: -6257.17264 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.12891 HOMO: -7.26544 LUMO: 0.41089 factor:1 | -1 (0.40942) | 1 | 1 |
| G: -6257.17264 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.09672 HOMO: -6.26406 LUMO: -0.85444 factor:1 | -1 (0.44161) | -1 | -1 |
| G: -6257.17264 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.09557 HOMO: -6.25318 LUMO: -0.79457 factor:1 | -1 (0.44276) | -1 | -1 |
| G: -6257.17264 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12520.82395 HOMO: -6.68040 LUMO: 0.41089 factor:1 | -1 (0.71438) | -1 | -1 |
| G: -6257.17264 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.29133 HOMO: -6.37835 LUMO: 0.37280 factor:1 | -1 (0.24700) | -1 | -1 |
| G: -6257.17264 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.41155 HOMO: -6.56067 LUMO: 0.62858 factor:1 | -1 (0.12678) | -1 | -1 |
| G: -6257.17264 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.48810 HOMO: -6.74026 LUMO: -0.04082 factor:1 | -1 (0.05023) | -1 | -1 |
| G: -6257.17264 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.38206 HOMO: -6.53617 LUMO: 0.35103 factor:1 | -1 (0.15627) | -1 | -1 |
| G: -6257.17264 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12520.95013 HOMO: -6.51985 LUMO: 0.25851 factor:1 | -1 (0.58820) | -1 | -1 |
| G: -6257.17264 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.37615 HOMO: -6.58788 LUMO: -1.98371 factor:1 | -1 (0.16218) | -1 | -1 |
| G: -6257.17264 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.30322 HOMO: -6.51441 LUMO: 0.29116 factor:1 | -1 (0.23511) | -1 | -1 |
| G: -6257.17264 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.08004 HOMO: -6.81101 LUMO: 0.35647 factor:1 | -1 (0.45829) | -1 | -1 |
| G: -6257.17264 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12520.99448 HOMO: -6.42733 LUMO: 0.10340 factor:1 | -1 (0.54385) | -1 | -1 |
| G: -6257.17264 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12520.64174 HOMO: -6.70761 LUMO: 0.28028 factor:1 | -1 (0.89659) | -1 | -1 |
| G: -6257.17264 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.38494 HOMO: -6.67495 LUMO: 0.01633 factor:1 | -1 (0.15339) | -1 | -1 |
| G: -6257.17264 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.07364 HOMO: -6.75387 LUMO: 0.15510 factor:1 | -1 (0.46469) | -1 | -1 |
| G: -6257.17264 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.24091 HOMO: -6.56067 LUMO: 0.35919 factor:1 | -1 (0.29742) | -1 | -1 |
| G: -6257.17264 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.43403 HOMO: -7.16748 LUMO: 0.21497 factor:1 | -1 (0.10430) | 1 | 1 |
| G: -6257.17264 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.66144 HOMO: -6.71849 LUMO: 0.26667 factor:1 | 1 (-0.12310) | -1 | -1 |
| G: -6257.17264 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.16610 HOMO: -6.69128 LUMO: 0.55783 factor:1 | 1 (-0.62777) | -1 | -1 |
| G: -6257.17264 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.10242 HOMO: -6.71305 LUMO: 0.45987 factor:1 | 1 (-0.56409) | -1 | -1 |
| G: -6257.17264 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.11293 HOMO: -5.90487 LUMO: -0.70750 factor:1 | 1 (-0.57460) | -1 | -1 |
| G: -6257.17264 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.76734 HOMO: -6.84638 LUMO: -0.72110 factor:1 | 1 (-0.22901) | -1 | -1 |
| G: -6257.17264 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.90438 HOMO: -6.66135 LUMO: -1.13471 factor:1 | 1 (-0.36605) | -1 | -1 |
| G: -6257.17264 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.83140 HOMO: -6.74026 LUMO: -0.64763 factor:1 | 1 (-0.29307) | -1 | -1 |
| G: -6257.17264 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.77567 HOMO: -6.69672 LUMO: -1.05036 factor:1 | 1 (-0.23734) | -1 | -1 |
| G: -6257.17264 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.54625 HOMO: -6.78924 LUMO: -1.03675 factor:1 | 1 (-0.00792) | -1 | -1 |
| G: -6257.17264 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.64500 HOMO: -6.81373 LUMO: -0.85988 factor:1 | 1 (-0.10667) | -1 | -1 |
| G: -6257.17264 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.81880 HOMO: -7.26544 LUMO: 0.91158 factor:1 | 1 (-0.28047) | 1 | 1 |
| G: -6257.17264 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.93611 HOMO: -6.64230 LUMO: -1.92929 factor:1 | 1 (-0.39778) | -1 | -1 |
| G: -6257.17264 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.87099 HOMO: -7.20830 LUMO: 0.11429 factor:1 | 1 (-0.33266) | 1 | 1 |
| G: -6257.17264 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.28226 HOMO: -7.17020 LUMO: 0.04898 factor:1 | 1 (-0.74393) | 1 | 1 |
| G: -6257.17264 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.59685 HOMO: -7.16476 LUMO: 0.04898 factor:1 | 1 (-1.05852) | 1 | 1 |
| G: -6257.17264 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.49753 HOMO: -6.59332 LUMO: -0.49253 factor:1 | 1 (-0.95920) | -1 | -1 |
| G: -6257.17264 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.28264 HOMO: -7.46953 LUMO: 0.84083 factor:1 | 1 (-0.74431) | 1 | 1 |
| G: -6257.17264 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.59933 HOMO: -7.39878 LUMO: 0.88709 factor:1 | 1 (-1.06100) | 1 | 1 |
| G: -6257.17264 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.39603 HOMO: -6.84094 LUMO: -0.61498 factor:1 | 1 (-0.85770) | -1 | -1 |
| G: -6257.17264 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.08694 HOMO: -6.03549 LUMO: -0.27211 factor:1 | 1 (-0.54861) | -1 | -1 |
| G: -6257.17264 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.57189 HOMO: -7.31170 LUMO: -0.64763 factor:1 | 1 (-2.03356) | 1 | 1 |
| G: -6257.17264 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.69528 HOMO: -6.88992 LUMO: -0.84627 factor:1 | 1 (-1.15695) | -1 | -1 |
| G: -6257.17264 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.44295 HOMO: -7.12666 LUMO: -0.09252 factor:1 | 1 (-0.90462) | 1 | 1 |
| G: -6257.17264 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.30410 HOMO: -6.70489 LUMO: -0.63675 factor:1 | 1 (-1.76577) | -1 | -1 |
| G: -6257.17264 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.60521 HOMO: -6.98788 LUMO: 0.86804 factor:1 | 1 (-1.06688) | -1 | -1 |
| G: -6257.17264 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.58257 HOMO: -6.80285 LUMO: -0.60954 factor:1 | 1 (-1.04424) | -1 | -1 |
| G: -6257.17264 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.38539 HOMO: -7.02054 LUMO: -0.74287 factor:1 | 1 (-0.84706) | -1 | -1 |
| G: -6257.17264 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.56417 HOMO: -7.03686 LUMO: -0.81090 factor:1 | 1 (-1.02584) | -1 | -1 |
| G: -6257.17264 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.58934 HOMO: -6.70489 LUMO: -1.00954 factor:1 | 1 (-1.05101) | -1 | -1 |
| G: -6257.17264 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.69413 HOMO: -7.69810 LUMO: 0.00544 factor:1 | 1 (-1.15580) | 1 | 1 |
| G: -6257.17264 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.28523 HOMO: -6.83550 LUMO: -0.11157 factor:1 | 1 (-0.74690) | -1 | -1 |
| G: -6257.17264 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.39241 HOMO: -6.76203 LUMO: -2.13609 factor:1 | 1 (-0.85408) | -1 | -1 |
| G: -6257.17264 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.30256 HOMO: -6.72121 LUMO: -2.62862 factor:1 | 1 (-0.76423) | -1 | -1 |
| G: -6257.17264 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.46583 HOMO: -6.48719 LUMO: -2.73474 factor:1 | 1 (-0.92750) | -1 | -1 |
| G: -6257.17264 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.41018 HOMO: -6.83006 LUMO: -0.00544 factor:1 | 1 (-0.87185) | -1 | -1 |
| G: -6257.17264 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.17611 HOMO: -6.84094 LUMO: -1.11022 factor:1 | 1 (-0.63778) | -1 | -1 |
| G: -6257.17264 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.14789 HOMO: -6.66951 LUMO: -1.23812 factor:1 | 1 (-0.60956) | -1 | -1 |
| G: -6257.17264 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12520.81581 HOMO: -6.78380 LUMO: -1.27894 factor:1 | -1 (0.72252) | -1 | -1 |
| G: -6257.17264 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12520.72553 HOMO: -6.50352 LUMO: -0.56055 factor:1 | -1 (0.81280) | -1 | -1 |
| G: -6257.17264 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.12842 HOMO: -7.77974 LUMO: -0.26395 factor:1 | -1 (0.40991) | 1 | 1 |
| G: -6257.17264 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.01106 HOMO: -7.01510 LUMO: -1.64085 factor:1 | -1 (0.52728) | -1 | -1 |
| G: -6257.17264 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.64194 HOMO: -6.59876 LUMO: -0.91158 factor:1 | 1 (-1.10361) | -1 | -1 |
| G: -6257.17264 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.31394 HOMO: -4.67219 LUMO: -0.67756 factor:1 | 1 (-0.77561) | -1 | -1 |
| G: -6257.17264 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12520.72142 HOMO: -6.70489 LUMO: -0.65579 factor:1 | -1 (0.81691) | -1 | -1 |
| G: -6257.17264 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.03982 HOMO: -6.62325 LUMO: -0.60409 factor:1 | -1 (0.49851) | -1 | -1 |
| G: -6257.17264 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.59707 HOMO: -6.20147 LUMO: 0.15238 factor:1 | 1 (-1.05874) | -1 | -1 |
| G: -6257.17264 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.60611 HOMO: -6.43549 LUMO: -0.07075 factor:1 | 1 (-1.06777) | -1 | -1 |
| G: -6257.17264 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.31415 HOMO: -7.02054 LUMO: 0.13061 factor:1 | 1 (-0.77582) | -1 | -1 |
| G: -6257.17264 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.80106 HOMO: -7.04503 LUMO: 0.30749 factor:1 | 1 (-0.26273) | -1 | -1 |
| G: -6257.17264 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.04800 HOMO: -6.74842 LUMO: -0.99594 factor:1 | 1 (-0.50967) | -1 | -1 |
| G: -6257.17264 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.38154 HOMO: -6.35658 LUMO: 0.41633 factor:1 | -1 (0.15679) | -1 | -1 |
| G: -6257.17264 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.22290 HOMO: -6.79740 LUMO: 0.56872 factor:1 | -1 (0.31543) | -1 | -1 |
| G: -6257.17264 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.26619 HOMO: -6.51713 LUMO: -0.05987 factor:1 | -1 (0.27214) | -1 | -1 |
| G: -6257.17264 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.31169 HOMO: -6.68040 LUMO: 0.34558 factor:1 | -1 (0.22664) | -1 | -1 |
| G: -6257.17264 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12520.97179 HOMO: -6.39740 LUMO: 0.50069 factor:1 | -1 (0.56654) | -1 | -1 |
| G: -6257.17264 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.08839 HOMO: -6.91713 LUMO: -0.97145 factor:1 | -1 (0.44994) | -1 | -1 |
| G: -6257.17264 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.23130 HOMO: -7.10761 LUMO: -0.27483 factor:1 | -1 (0.30703) | 1 | -1 |
| G: -6257.17264 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.26377 HOMO: -6.98788 LUMO: 0.40273 factor:1 | -1 (0.27456) | -1 | -1 |
| G: -6257.17264 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.30820 HOMO: -6.87087 LUMO: 0.28572 factor:1 | 1 (-0.76986) | -1 | -1 |
| G: -6257.17264 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.40931 HOMO: -7.36612 LUMO: -0.12245 factor:1 | 1 (-0.87098) | 1 | 1 |
| G: -6257.17264 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.19854 HOMO: -6.72938 LUMO: 0.33742 factor:1 | -1 (0.33979) | -1 | -1 |
| G: -6257.17264 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.35161 HOMO: -7.32531 LUMO: 0.07619 factor:1 | -1 (0.18672) | 1 | 1 |
| G: -6257.17264 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.06871 HOMO: -6.87087 LUMO: -0.08436 factor:1 | 1 (-0.53038) | -1 | -1 |
| G: -6257.17264 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.04452 HOMO: -6.67495 LUMO: 0.85988 factor:1 | 1 (-0.50619) | -1 | -1 |
| G: -6257.17264 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.07567 HOMO: -6.96339 LUMO: 0.65307 factor:1 | 1 (-0.53734) | -1 | -1 |
| G: -6257.17264 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.23423 HOMO: -6.58516 LUMO: -0.78641 factor:1 | 1 (-0.69590) | -1 | -1 |
| G: -6257.17264 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.89606 HOMO: -6.56883 LUMO: 0.44355 factor:1 | 1 (-2.35773) | -1 | -1 |
| G: -6257.17264 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.11518 HOMO: -6.68312 LUMO: 0.43538 factor:1 | 1 (-1.57685) | -1 | -1 |
| G: -6257.17264 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.88746 HOMO: -6.81917 LUMO: 0.20681 factor:1 | 1 (-2.34913) | -1 | -1 |
| G: -6257.17264 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.58035 HOMO: -6.91169 LUMO: 0.08163 factor:1 | 1 (-2.04202) | -1 | -1 |
| G: -6257.17264 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.77128 HOMO: -4.88444 LUMO: -0.49253 factor:1 | 1 (-1.23295) | -1 | -1 |
| G: -6257.17264 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.02312 HOMO: -6.42189 LUMO: 0.64763 factor:1 | 1 (-1.48479) | -1 | -1 |
| G: -6257.17264 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.35826 HOMO: -6.24501 LUMO: 0.55783 factor:1 | 1 (-1.81992) | -1 | -1 |
| G: -6257.17264 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.30741 HOMO: -6.41372 LUMO: 0.29388 factor:1 | 1 (-0.76908) | -1 | -1 |
| G: -6257.17264 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.08291 HOMO: -5.67902 LUMO: 1.77690 factor:1 | 1 (-0.54458) | -1 | -1 |
| G: -6257.17264 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.85461 HOMO: -6.55794 LUMO: 0.05170 factor:1 | 1 (-0.31628) | -1 | -1 |
| G: -6257.17264 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.55727 HOMO: -6.52801 LUMO: 0.25851 factor:1 | 1 (-0.01894) | -1 | -1 |
| G: -6257.17264 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.02626 HOMO: -7.08857 LUMO: 0.11157 factor:1 | 1 (-0.48793) | 1 | 1 |
| G: -6257.17264 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12520.85138 HOMO: -6.58243 LUMO: 0.75648 factor:1 | -1 (0.68695) | -1 | -1 |
| G: -6257.17264 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12520.88790 HOMO: -7.22190 LUMO: 0.45171 factor:1 | -1 (0.65043) | 1 | 1 |
| G: -6257.17264 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.19171 HOMO: -6.47087 LUMO: 0.00000 factor:1 | -1 (0.34662) | -1 | -1 |
| G: -6257.17264 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.07617 HOMO: -6.78652 LUMO: 1.32247 factor:1 | -1 (0.46216) | -1 | -1 |
| G: -6257.17264 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12520.86537 HOMO: -6.74026 LUMO: 1.45309 factor:1 | -1 (0.67296) | -1 | -1 |
| G: -6257.17264 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.21824 HOMO: -6.69944 LUMO: 0.76464 factor:1 | -1 (0.32009) | -1 | -1 |
| G: -6257.17264 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12520.58871 HOMO: -6.62325 LUMO: 0.64763 factor:1 | -1 (0.94962) | -1 | -1 |
| G: -6257.17264 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12520.44783 HOMO: -6.45182 LUMO: 0.49253 factor:1 | -1 (1.09050) | -1 | -1 |
| G: -6257.17264 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.18450 HOMO: -7.14843 LUMO: 0.62586 factor:1 | -1 (0.35383) | 1 | 1 |
| G: -6257.17264 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.34480 HOMO: -6.87087 LUMO: 1.53200 factor:1 | -1 (0.19353) | -1 | -1 |
| G: -6257.17264 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.15830 HOMO: -6.54978 LUMO: 0.45171 factor:1 | -1 (0.38003) | -1 | -1 |
| G: -6257.17264 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.22714 HOMO: -6.63686 LUMO: 0.80001 factor:1 | -1 (0.31119) | -1 | -1 |
| G: -6257.17264 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.06975 HOMO: -7.00693 LUMO: 1.56193 factor:1 | -1 (0.46858) | -1 | -1 |
| G: -6257.17264 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.14504 HOMO: -6.02460 LUMO: 1.72792 factor:1 | -1 (0.39329) | -1 | -1 |
| G: -6257.17264 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.00194 HOMO: -6.36746 LUMO: -1.20002 factor:1 | -1 (0.53639) | -1 | -1 |
| G: -6257.17264 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.16994 HOMO: -7.26816 LUMO: -1.06397 factor:1 | -1 (0.36839) | 1 | 1 |
| G: -6257.17264 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12520.84000 HOMO: -7.34707 LUMO: -1.09662 factor:1 | -1 (0.69833) | 1 | 1 |
| G: -6257.17264 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.22940 HOMO: -7.93212 LUMO: -0.13606 factor:1 | -1 (0.30893) | 1 | 1 |
| G: -6257.17264 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.87594 HOMO: -6.80285 LUMO: 0.58504 factor:1 | 1 (-0.33761) | -1 | -1 |
| G: -6257.17264 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.52913 HOMO: -7.12938 LUMO: 0.32926 factor:1 | -1 (0.00920) | 1 | -1 |
| G: -6257.17264 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.46840 HOMO: -6.86815 LUMO: -1.30070 factor:1 | -1 (0.06993) | -1 | -1 |
| G: -6257.17264 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.70008 HOMO: -6.99333 LUMO: -1.03947 factor:1 | 1 (-0.16174) | -1 | -1 |
| G: -6257.17264 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12520.67206 HOMO: -7.56749 LUMO: -0.11157 factor:1 | -1 (0.86627) | 1 | 1 |
| G: -6257.17264 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12520.81837 HOMO: -7.57293 LUMO: -0.07891 factor:1 | -1 (0.71996) | 1 | 1 |
| G: -6257.17264 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12520.58835 HOMO: -7.30626 LUMO: 0.27211 factor:1 | -1 (0.94998) | 1 | 1 |
| G: -6257.17264 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12520.71219 HOMO: -7.77974 LUMO: 0.27211 factor:1 | -1 (0.82614) | 1 | 1 |
| G: -6257.17264 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12520.34840 HOMO: -7.11578 LUMO: 0.19864 factor:1 | -1 (1.18993) | 1 | 1 |
| G: -6257.17264 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12520.79644 HOMO: -7.71171 LUMO: 0.57688 factor:1 | -1 (0.74189) | 1 | 1 |
| G: -6257.17264 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.41063 HOMO: -7.83688 LUMO: 0.37824 factor:1 | -1 (0.12770) | 1 | 1 |
| G: -6257.17264 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.45985 HOMO: -6.94979 LUMO: -1.66534 factor:1 | -1 (0.07848) | -1 | -1 |
| G: -6257.17264 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12520.22299 HOMO: -6.97156 LUMO: -1.13199 factor:1 | -1 (1.31534) | -1 | -1 |
| G: -6257.17264 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12520.26223 HOMO: -6.91441 LUMO: -1.08301 factor:1 | -1 (1.27611) | -1 | -1 |
| G: -6257.17264 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.55009 HOMO: -6.71849 LUMO: -0.74831 factor:1 | 1 (-0.01176) | -1 | -1 |
| G: -6257.17264 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.48652 HOMO: -7.09401 LUMO: -1.77690 factor:1 | -1 (0.05181) | -1 | -1 |
| G: -6257.17264 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12520.23831 HOMO: -6.97156 LUMO: -1.45037 factor:1 | -1 (1.30002) | -1 | -1 |
| G: -6257.17264 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12520.17224 HOMO: -7.22462 LUMO: -1.11295 factor:1 | -1 (1.36609) | 1 | 1 |
| G: -6257.17264 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12519.76121 HOMO: -7.85321 LUMO: 0.16599 factor:1 | -1 (1.77712) | 1 | 1 |
| G: -6257.17264 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12519.74943 HOMO: -7.71987 LUMO: 0.55511 factor:1 | -1 (1.78890) | 1 | 1 |
| G: -6257.17264 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12519.98584 HOMO: -7.63551 LUMO: 0.14422 factor:1 | -1 (1.55249) | 1 | 1 |
| G: -6257.17264 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.36091 HOMO: -6.98788 LUMO: -0.80546 factor:1 | -1 (0.17742) | -1 | -1 |
| G: -6257.17264 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.46875 HOMO: -6.98788 LUMO: -1.16737 factor:1 | -1 (0.06958) | -1 | -1 |
| G: -6257.17264 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.57346 HOMO: -6.56611 LUMO: -1.60819 factor:1 | 1 (-0.03513) | -1 | -1 |
| G: -6257.17264 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.58103 HOMO: -6.95251 LUMO: 0.66396 factor:1 | 1 (-0.04269) | -1 | -1 |
| G: -6257.17264 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.39675 HOMO: -7.35252 LUMO: 0.49797 factor:1 | -1 (0.14158) | 1 | 1 |
| G: -6257.17264 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.22173 HOMO: -6.90897 LUMO: -0.81090 factor:1 | -1 (0.31660) | -1 | -1 |
| G: -6257.17264 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.26886 HOMO: -7.04503 LUMO: -1.08301 factor:1 | -1 (0.26947) | -1 | -1 |
| G: -6257.17264 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.32771 HOMO: -6.92530 LUMO: -1.29526 factor:1 | -1 (0.21062) | -1 | -1 |
| G: -6257.17264 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.19694 HOMO: -6.93074 LUMO: -1.25444 factor:1 | -1 (0.34139) | -1 | -1 |
| G: -6257.17264 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.04793 HOMO: -6.73482 LUMO: -0.62042 factor:1 | -1 (0.49040) | -1 | -1 |
| G: -6257.17264 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12520.87606 HOMO: -7.67633 LUMO: 0.59593 factor:1 | -1 (0.66227) | 1 | 1 |
| G: -6257.17264 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12520.52231 HOMO: -7.39061 LUMO: -0.19320 factor:1 | -1 (1.01602) | 1 | 1 |
| G: -6257.17264 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12520.96232 HOMO: -7.55388 LUMO: -0.20136 factor:1 | -1 (0.57601) | 1 | 1 |
| G: -6257.17264 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.92920 HOMO: -7.14027 LUMO: -0.99866 factor:1 | 1 (-0.39086) | 1 | 1 |
| G: -6257.17264 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.24115 HOMO: -6.75931 LUMO: -0.73199 factor:1 | 1 (-0.70282) | -1 | -1 |
| G: -6257.17264 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.44921 HOMO: -5.45044 LUMO: -0.18776 factor:1 | -1 (0.08912) | -1 | -1 |
| G: -6257.17264 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.72715 HOMO: -6.70761 LUMO: -0.84083 factor:1 | 1 (-0.18882) | -1 | -1 |
| G: -6257.17264 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12520.59663 HOMO: -6.05453 LUMO: -1.06669 factor:1 | -1 (0.94170) | -1 | -1 |
| G: -6257.17264 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12520.65255 HOMO: -6.86815 LUMO: -0.98233 factor:1 | -1 (0.88579) | -1 | -1 |
| G: -6257.17264 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12520.55924 HOMO: -6.73210 LUMO: -0.95240 factor:1 | -1 (0.97909) | -1 | -1 |
| G: -6257.17264 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12520.36843 HOMO: -5.89671 LUMO: -1.05036 factor:1 | -1 (1.16990) | -1 | -1 |
| G: -6257.17264 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12520.93723 HOMO: -7.61102 LUMO: 0.33470 factor:1 | -1 (0.60110) | 1 | 1 |
| G: -6257.17264 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12520.82890 HOMO: -7.51034 LUMO: 0.23674 factor:1 | -1 (0.70943) | 1 | 1 |
| G: -6257.17264 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.28263 HOMO: -7.41510 LUMO: 0.62858 factor:1 | -1 (0.25571) | 1 | 1 |
| G: -6257.17264 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.37245 HOMO: -6.76203 LUMO: -1.72792 factor:1 | -1 (0.16588) | -1 | -1 |
| G: -6257.17264 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.98441 HOMO: -6.60420 LUMO: -0.45715 factor:1 | 1 (-0.44608) | -1 | -1 |
| G: -6257.17264 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.24923 HOMO: -6.59060 LUMO: -0.58232 factor:1 | 1 (-0.71090) | -1 | -1 |
| G: -6257.17264 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.19440 HOMO: -7.43687 LUMO: -0.76736 factor:1 | 1 (-0.65607) | 1 | 1 |
| G: -6257.17264 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.41198 HOMO: -6.08719 LUMO: -0.48708 factor:1 | 1 (-0.87365) | -1 | -1 |
| G: -6257.17264 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.81047 HOMO: -5.88854 LUMO: -0.05714 factor:1 | 1 (-0.27214) | -1 | -1 |
| G: -6257.17264 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.58247 HOMO: -7.34435 LUMO: -0.71838 factor:1 | 1 (-0.04414) | 1 | 1 |
| G: -6257.17264 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.53185 HOMO: -7.46408 LUMO: -0.63130 factor:1 | -1 (0.00648) | 1 | 1 |
| G: -6257.17264 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.46959 HOMO: -7.00965 LUMO: -1.24900 factor:1 | -1 (0.06874) | -1 | -1 |
| G: -6257.17264 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.82887 HOMO: -6.91169 LUMO: -0.88981 factor:1 | 1 (-0.29054) | -1 | -1 |
| G: -6257.17264 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.74184 HOMO: -6.78652 LUMO: -0.82178 factor:1 | 1 (-0.20351) | -1 | -1 |
| G: -6257.17264 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.45104 HOMO: -7.80423 LUMO: 0.87076 factor:1 | -1 (0.08729) | 1 | 1 |
| G: -6257.17264 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.10738 HOMO: -6.97700 LUMO: -1.00954 factor:1 | -1 (0.43095) | -1 | -1 |
| G: -6257.17264 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.78345 HOMO: -6.92530 LUMO: -0.88165 factor:1 | 1 (-0.24512) | -1 | -1 |
| G: -6257.17264 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.42434 HOMO: -7.14571 LUMO: -1.04492 factor:1 | -1 (0.11399) | 1 | 1 |
| G: -6257.17264 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.27369 HOMO: -7.49674 LUMO: 0.34558 factor:1 | 1 (-0.73536) | 1 | 1 |
| G: -6257.17264 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.45916 HOMO: -6.44094 LUMO: -1.20819 factor:1 | 1 (-0.92083) | -1 | -1 |
| G: -6257.17264 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.45233 HOMO: -6.47359 LUMO: -1.14016 factor:1 | 1 (-1.91399) | -1 | -1 |
| G: -6257.17264 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.61068 HOMO: -6.61237 LUMO: -0.87076 factor:1 | 1 (-1.07235) | -1 | -1 |
| G: -6257.17264 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.54016 HOMO: -6.73754 LUMO: -1.09662 factor:1 | 1 (-2.00183) | -1 | -1 |
| G: -6257.17264 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.47974 HOMO: -6.97700 LUMO: 0.13061 factor:1 | 1 (-0.94141) | -1 | -1 |
| G: -6257.17264 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.37858 HOMO: -6.82734 LUMO: 0.59865 factor:1 | 1 (-1.84025) | -1 | -1 |
| G: -6257.17264 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.39815 HOMO: -6.86543 LUMO: -0.91430 factor:1 | 1 (-1.85982) | -1 | -1 |
| G: -6257.17264 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.12405 HOMO: -6.74298 LUMO: 0.28028 factor:1 | 1 (-1.58572) | -1 | -1 |
| G: -6257.17264 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.19010 HOMO: -6.75387 LUMO: 0.19592 factor:1 | 1 (-0.65177) | -1 | -1 |
| G: -6257.17264 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.30822 HOMO: -7.05591 LUMO: 0.10612 factor:1 | 1 (-0.76989) | -1 | -1 |
| G: -6257.17264 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.88647 HOMO: -6.86543 LUMO: 0.49253 factor:1 | 1 (-0.34814) | -1 | -1 |
| G: -6257.17264 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.44401 HOMO: -6.11440 LUMO: -1.12655 factor:1 | 1 (-0.90568) | -1 | -1 |
| G: -6257.17264 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.93195 HOMO: -6.77291 LUMO: -1.02859 factor:1 | 1 (-2.39362) | -1 | -1 |
| G: -6257.17264 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.89900 HOMO: -6.54978 LUMO: 0.29116 factor:1 | 1 (-2.36067) | -1 | -1 |
| G: -6257.17264 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.98254 HOMO: -7.18108 LUMO: 0.00000 factor:1 | 1 (-2.44421) | 1 | 1 |
| G: -6257.17264 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12524.44698 HOMO: -6.86271 LUMO: -1.15376 factor:1 | 1 (-2.90865) | -1 | -1 |
| G: -6257.17264 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.15485 HOMO: -6.78108 LUMO: -1.22723 factor:1 | 1 (-1.61652) | -1 | -1 |
| G: -6257.17264 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.74330 HOMO: -6.40828 LUMO: 0.02449 factor:1 | 1 (-2.20497) | -1 | -1 |
| G: -6257.17264 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12524.03043 HOMO: -6.43821 LUMO: 0.09796 factor:1 | 1 (-2.49210) | -1 | -1 |
| G: -6257.17264 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.25072 HOMO: -6.99877 LUMO: 0.40545 factor:1 | 1 (-1.71239) | -1 | -1 |
| G: -6257.17264 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.72581 HOMO: -6.68856 LUMO: 0.19320 factor:1 | 1 (-1.18748) | -1 | -1 |
| G: -6257.17264 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.67762 HOMO: -7.11034 LUMO: 0.31293 factor:1 | 1 (-1.13929) | 1 | 1 |
| G: -6257.17264 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.39013 HOMO: -6.92530 LUMO: -0.85444 factor:1 | 1 (-0.85180) | -1 | -1 |
| G: -6257.17264 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.40376 HOMO: -6.60148 LUMO: -0.59865 factor:1 | 1 (-0.86543) | -1 | -1 |
| G: -6257.17264 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.29108 HOMO: -6.72938 LUMO: 0.30749 factor:1 | 1 (-0.75275) | -1 | -1 |
| G: -6257.17264 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.43516 HOMO: -7.31170 LUMO: 0.06803 factor:1 | 1 (-0.89683) | 1 | 1 |
| G: -6257.17264 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12524.04883 HOMO: -7.09129 LUMO: -0.04626 factor:1 | 1 (-2.51050) | 1 | 1 |
| G: -6257.17264 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.25368 HOMO: -6.38379 LUMO: -0.76736 factor:1 | 1 (-1.71535) | -1 | -1 |
| G: -6257.17264 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12524.07400 HOMO: -6.13617 LUMO: -0.63947 factor:1 | 1 (-2.53567) | -1 | -1 |
| G: -6257.17264 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12524.18385 HOMO: -6.92258 LUMO: 0.37007 factor:1 | 1 (-2.64552) | -1 | -1 |
| G: -6257.17264 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.33308 HOMO: -6.35930 LUMO: 0.41361 factor:1 | 1 (-1.79475) | -1 | -1 |
| G: -6257.17264 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12524.02298 HOMO: -6.60420 LUMO: 0.26667 factor:1 | 1 (-2.48464) | -1 | -1 |
| G: -6257.17264 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.07460 HOMO: -6.04909 LUMO: 1.82588 factor:1 | 1 (-1.53627) | -1 | -1 |
| G: -6257.17264 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.27254 HOMO: -6.69672 LUMO: 1.72520 factor:1 | 1 (-1.73421) | -1 | -1 |
| G: -6257.17264 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.37452 HOMO: -6.50080 LUMO: 0.29116 factor:1 | -1 (0.16381) | -1 | -1 |
| G: -6257.17264 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.16730 HOMO: -6.60692 LUMO: -0.43266 factor:1 | -1 (0.37103) | -1 | -1 |
| G: -6257.17264 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.30456 HOMO: -6.93890 LUMO: 0.39729 factor:1 | -1 (0.23377) | -1 | -1 |
| G: -6257.17264 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.19543 HOMO: -6.52801 LUMO: -0.47076 factor:1 | 1 (-0.65710) | -1 | -1 |
| G: -6257.17264 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.98688 HOMO: -6.41100 LUMO: 0.30477 factor:1 | 1 (-0.44855) | -1 | -1 |
| G: -6257.17264 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.25317 HOMO: -6.37291 LUMO: -0.80001 factor:1 | 1 (-0.71484) | -1 | -1 |
| G: -6257.17264 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.11018 HOMO: -6.51985 LUMO: 1.44765 factor:1 | 1 (-0.57185) | -1 | -1 |
| G: -6257.17264 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.85153 HOMO: -6.64774 LUMO: 0.04626 factor:1 | 1 (-0.31320) | -1 | -1 |
| G: -6257.17264 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.97635 HOMO: -6.65863 LUMO: 0.29933 factor:1 | 1 (-0.43802) | -1 | -1 |
| G: -6257.17264 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.07845 HOMO: -7.09673 LUMO: 0.28300 factor:1 | 1 (-0.54012) | 1 | 1 |
| G: -6257.17264 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.22100 HOMO: -6.57155 LUMO: -1.11567 factor:1 | 1 (-1.68267) | -1 | -1 |
| G: -6257.17264 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12524.12845 HOMO: -6.38379 LUMO: -0.60681 factor:1 | 1 (-2.59012) | -1 | -1 |
| G: -6257.17264 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12524.18613 HOMO: -6.60148 LUMO: 0.18232 factor:1 | 1 (-2.64780) | -1 | -1 |
| G: -6257.17264 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.70961 HOMO: -6.96067 LUMO: -0.52246 factor:1 | 1 (-2.17128) | -1 | -1 |
| G: -6257.17264 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.96208 HOMO: -6.57427 LUMO: -0.84627 factor:1 | 1 (-1.42375) | -1 | -1 |
| G: -6257.17264 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.15469 HOMO: -6.59332 LUMO: -0.98233 factor:1 | 1 (-1.61636) | -1 | -1 |
| G: -6257.17264 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.34944 HOMO: -6.20692 LUMO: -0.27483 factor:1 | 1 (-1.81111) | -1 | -1 |
| G: -6257.17264 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.57389 HOMO: -6.81373 LUMO: 0.74559 factor:1 | 1 (-1.03556) | -1 | -1 |
| G: -6257.17264 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.28907 HOMO: -6.60420 LUMO: 0.54695 factor:1 | -1 (0.24926) | -1 | -1 |
| G: -6257.17264 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.11597 HOMO: -6.58788 LUMO: -0.31021 factor:1 | 1 (-0.57764) | -1 | -1 |
| G: -6257.17264 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.33824 HOMO: -6.72938 LUMO: 0.64763 factor:1 | 1 (-0.79991) | -1 | -1 |
| G: -6257.17264 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.92623 HOMO: -6.86815 LUMO: 0.32109 factor:1 | 1 (-0.38790) | -1 | -1 |
| G: -6257.17264 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.26936 HOMO: -6.63141 LUMO: 0.18776 factor:1 | 1 (-0.73103) | -1 | -1 |
| G: -6257.17264 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.54926 HOMO: -7.18653 LUMO: 0.09524 factor:1 | 1 (-1.01093) | 1 | 1 |
| G: -6257.17264 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.28270 HOMO: -6.83550 LUMO: 0.03537 factor:1 | 1 (-0.74437) | -1 | -1 |
| G: -6257.17264 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.93959 HOMO: -7.47769 LUMO: 0.40817 factor:1 | 1 (-0.40126) | 1 | 1 |
| G: -6257.17264 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.58608 HOMO: -6.57971 LUMO: -0.63675 factor:1 | 1 (-1.04775) | -1 | -1 |
| G: -6257.17264 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.38948 HOMO: -6.74842 LUMO: -0.16327 factor:1 | 1 (-0.85114) | -1 | -1 |
| G: -6257.17264 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.38616 HOMO: -7.07224 LUMO: 0.61770 factor:1 | 1 (-0.84783) | 1 | 1 |
| G: -6257.17264 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.61239 HOMO: -6.83006 LUMO: 0.54695 factor:1 | 1 (-1.07406) | -1 | -1 |
| G: -6257.17264 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.75329 HOMO: -6.60148 LUMO: 1.23540 factor:1 | 1 (-1.21496) | -1 | -1 |
| G: -6257.17264 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.26011 HOMO: -6.99061 LUMO: 0.41089 factor:1 | 1 (-0.72178) | -1 | -1 |
| G: -6257.17264 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.51138 HOMO: -6.63686 LUMO: 0.85172 factor:1 | 1 (-0.97305) | -1 | -1 |
| G: -6257.17264 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.52638 HOMO: -6.50624 LUMO: 0.12517 factor:1 | 1 (-0.98805) | -1 | -1 |
| G: -6257.17264 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.43054 HOMO: -6.35658 LUMO: 0.36463 factor:1 | 1 (-0.89221) | -1 | -1 |
| G: -6257.17264 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.28116 HOMO: -6.34570 LUMO: 0.65035 factor:1 | -1 (0.25717) | -1 | -1 |
| G: -6257.17264 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12520.93492 HOMO: -6.63141 LUMO: 1.25717 factor:1 | -1 (0.60341) | -1 | -1 |
| G: -6257.17264 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.27778 HOMO: -6.91441 LUMO: 1.32792 factor:1 | -1 (0.26055) | -1 | -1 |
| G: -6257.17264 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.67617 HOMO: -7.15387 LUMO: 0.64219 factor:1 | 1 (-1.13784) | 1 | 1 |
| G: -6257.17264 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.27347 HOMO: -7.17836 LUMO: 0.60409 factor:1 | 1 (-0.73514) | 1 | 1 |
| G: -6257.17264 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.47742 HOMO: -6.92258 LUMO: 0.49525 factor:1 | 1 (-0.93909) | -1 | -1 |
| G: -6257.17264 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.93477 HOMO: -6.31032 LUMO: 0.48708 factor:1 | 1 (-0.39644) | -1 | -1 |
| G: -6257.17264 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.24109 HOMO: -6.49808 LUMO: 0.31021 factor:1 | 1 (-0.70276) | -1 | -1 |
| G: -6257.17264 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.28558 HOMO: -6.48447 LUMO: 0.37552 factor:1 | 1 (-0.74725) | -1 | -1 |
| G: -6257.17264 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.20602 HOMO: -6.66135 LUMO: -1.08301 factor:1 | 1 (-0.66769) | -1 | -1 |
| G: -6257.17264 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.92446 HOMO: -6.33481 LUMO: -0.51974 factor:1 | 1 (-0.38613) | -1 | -1 |
| G: -6257.17264 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.02356 HOMO: -6.76475 LUMO: -0.15238 factor:1 | 1 (-0.48523) | -1 | -1 |
| G: -6257.17264 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.74288 HOMO: -6.93346 LUMO: -0.10885 factor:1 | 1 (-0.20455) | -1 | -1 |
| G: -6257.17264 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.16985 HOMO: -7.19741 LUMO: 0.73199 factor:1 | 1 (-0.63152) | 1 | 1 |
| G: -6257.17264 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.44227 HOMO: -6.82734 LUMO: 0.88437 factor:1 | -1 (0.09606) | -1 | -1 |
| G: -6257.17264 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.36690 HOMO: -7.01237 LUMO: 0.02721 factor:1 | -1 (0.17143) | -1 | -1 |
| G: -6257.17264 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12520.86376 HOMO: -6.39195 LUMO: 1.46941 factor:1 | -1 (0.67457) | -1 | -1 |
| G: -6257.17264 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.15043 HOMO: -6.53890 LUMO: 1.32792 factor:1 | -1 (0.38790) | -1 | -1 |
| G: -6257.17264 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.47558 HOMO: -6.82734 LUMO: 1.98099 factor:1 | -1 (0.06275) | -1 | -1 |
| G: -6257.17264 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.55945 HOMO: -6.74570 LUMO: 1.68983 factor:1 | 1 (-0.02112) | -1 | -1 |
| G: -6257.17264 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.74087 HOMO: -6.41100 LUMO: 1.39050 factor:1 | 1 (-0.20253) | -1 | -1 |
| G: -6257.17264 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.91254 HOMO: -5.92664 LUMO: 1.65989 factor:1 | 1 (-0.37421) | -1 | -1 |
| G: -6257.17264 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.39217 HOMO: -6.07630 LUMO: 1.54833 factor:1 | 1 (-0.85384) | -1 | -1 |
| G: -6257.17264 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.45666 HOMO: -6.45998 LUMO: 0.68573 factor:1 | 1 (-0.91833) | -1 | -1 |
| G: -6257.17264 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.02263 HOMO: -6.52801 LUMO: 0.41361 factor:1 | 1 (-1.48430) | -1 | -1 |
| G: -6257.17264 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.02990 HOMO: -6.77564 LUMO: 0.42178 factor:1 | 1 (-1.49156) | -1 | -1 |
| G: -6257.17264 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.24746 HOMO: -6.56339 LUMO: 1.65717 factor:1 | 1 (-0.70913) | -1 | -1 |
| G: -6257.17264 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.79479 HOMO: -5.85861 LUMO: 1.90752 factor:1 | 1 (-1.25646) | -1 | -1 |
| G: -6257.17264 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.49862 HOMO: -6.77019 LUMO: -2.48440 factor:1 | 1 (-0.96029) | -1 | -1 |
| G: -6257.17264 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.13491 HOMO: -6.53890 LUMO: -1.82588 factor:1 | 1 (-0.59658) | -1 | -1 |
| G: -6257.17264 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.29655 HOMO: -6.50352 LUMO: -1.66806 factor:1 | 1 (-0.75822) | -1 | -1 |
| G: -6257.17264 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.99883 HOMO: -6.90625 LUMO: 0.43538 factor:1 | 1 (-0.46050) | -1 | -1 |
| G: -6257.17264 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.28585 HOMO: -6.85455 LUMO: 0.53062 factor:1 | 1 (-0.74752) | -1 | -1 |
| G: -6257.17264 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.21506 HOMO: -6.49536 LUMO: 0.31021 factor:1 | -1 (0.32327) | -1 | -1 |
| G: -6257.17264 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.29101 HOMO: -4.97696 LUMO: -0.09252 factor:1 | -1 (0.24732) | -1 | -1 |
| G: -6257.17264 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.22760 HOMO: -5.31166 LUMO: 0.34286 factor:1 | -1 (0.31073) | -1 | -1 |
| G: -6257.17264 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.15109 HOMO: -6.42461 LUMO: 0.74287 factor:1 | -1 (0.38725) | -1 | -1 |
| G: -6257.17264 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.16891 HOMO: -6.59604 LUMO: 0.62858 factor:1 | -1 (0.36942) | -1 | -1 |
| G: -6257.17264 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.05182 HOMO: -6.45998 LUMO: -0.61770 factor:1 | -1 (0.48651) | -1 | -1 |
| G: -6257.17264 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.45805 HOMO: -6.75659 LUMO: -0.34014 factor:1 | 1 (-0.91972) | -1 | -1 |
| G: -6257.17264 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.01395 HOMO: -6.63958 LUMO: 0.36191 factor:1 | 1 (-1.47562) | -1 | -1 |
| G: -6257.17264 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.74042 HOMO: -5.92936 LUMO: -0.67484 factor:1 | 1 (-1.20209) | -1 | -1 |
| G: -6257.17264 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.12012 HOMO: -5.67630 LUMO: 1.80956 factor:1 | -1 (0.41821) | -1 | -1 |
| G: -6257.17264 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.69291 HOMO: -6.50352 LUMO: -0.78369 factor:1 | 1 (-1.15458) | -1 | -1 |
| G: -6257.17264 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.39290 HOMO: -6.35930 LUMO: -0.75648 factor:1 | 1 (-0.85457) | -1 | -1 |
| G: -6257.17264 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.48886 HOMO: -6.74298 LUMO: 0.48980 factor:1 | -1 (0.04947) | -1 | -1 |
| G: -6257.17264 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.54763 HOMO: -6.85183 LUMO: 0.15510 factor:1 | 1 (-1.00930) | -1 | -1 |
| G: -6257.17264 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.78378 HOMO: -6.90897 LUMO: 0.26123 factor:1 | 1 (-0.24545) | -1 | -1 |
| G: -6257.17264 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.11225 HOMO: -6.85999 LUMO: 0.47892 factor:1 | 1 (-0.57392) | -1 | -1 |
| G: -6257.17264 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.15930 HOMO: -6.69944 LUMO: 0.57416 factor:1 | -1 (0.37903) | -1 | -1 |
| G: -6257.17264 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.19441 HOMO: -6.74026 LUMO: 0.69933 factor:1 | -1 (0.34392) | -1 | -1 |
| G: -6257.17264 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.23299 HOMO: -6.52801 LUMO: 0.75376 factor:1 | -1 (0.30534) | -1 | -1 |
| G: -6257.17264 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.31601 HOMO: -7.05863 LUMO: 0.44627 factor:1 | -1 (0.22232) | -1 | -1 |
| G: -6257.17264 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.15661 HOMO: -6.96339 LUMO: 0.48164 factor:1 | -1 (0.38172) | -1 | -1 |
| G: -6257.17264 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.26423 HOMO: -6.95795 LUMO: 0.44355 factor:1 | -1 (0.27410) | -1 | -1 |
| G: -6257.17264 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.38249 HOMO: -6.36746 LUMO: 0.58777 factor:1 | -1 (0.15584) | -1 | -1 |
| G: -6257.17264 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12520.99631 HOMO: -6.69400 LUMO: 0.40545 factor:1 | -1 (0.54202) | -1 | -1 |
| G: -6257.17264 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.27751 HOMO: -6.30760 LUMO: -0.66668 factor:1 | -1 (0.26082) | -1 | -1 |
| G: -6257.17264 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12520.97764 HOMO: -6.53617 LUMO: -0.64491 factor:1 | -1 (0.56069) | -1 | -1 |
| G: -6257.17264 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.18763 HOMO: -6.80829 LUMO: 0.17415 factor:1 | -1 (0.35070) | -1 | -1 |
| G: -6257.17264 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.03413 HOMO: -6.80285 LUMO: 0.73471 factor:1 | -1 (0.50420) | -1 | -1 |
| G: -6257.17264 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.14597 HOMO: -6.43821 LUMO: 0.21769 factor:1 | -1 (0.39236) | -1 | -1 |
| G: -6257.17264 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.32722 HOMO: -6.98788 LUMO: 0.10885 factor:1 | -1 (0.21111) | -1 | -1 |
| G: -6257.17264 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.32118 HOMO: -7.15115 LUMO: 0.40817 factor:1 | -1 (0.21715) | 1 | 1 |
| G: -6257.17264 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.29762 HOMO: -6.00011 LUMO: -0.98505 factor:1 | -1 (0.24071) | -1 | -1 |
| G: -6257.17264 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.35191 HOMO: -6.16882 LUMO: -0.77825 factor:1 | -1 (0.18643) | -1 | -1 |
| G: -6257.17264 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.10613 HOMO: -6.30760 LUMO: 0.34831 factor:1 | -1 (0.43220) | -1 | -1 |
| G: -6257.17264 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12520.99032 HOMO: -6.64502 LUMO: 0.63403 factor:1 | -1 (0.54801) | -1 | -1 |
| G: -6257.17264 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.11903 HOMO: -6.93618 LUMO: 0.96600 factor:1 | -1 (0.41930) | -1 | -1 |
| G: -6257.17264 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.20641 HOMO: -6.45182 LUMO: 0.16327 factor:1 | -1 (0.33192) | -1 | -1 |
| G: -6257.17264 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.23065 HOMO: -6.99605 LUMO: 0.20953 factor:1 | -1 (0.30768) | -1 | -1 |
| G: -6257.17264 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.84772 HOMO: -6.72665 LUMO: 0.32654 factor:1 | 1 (-0.30939) | -1 | -1 |
| G: -6257.17264 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.84225 HOMO: -6.38379 LUMO: 0.45443 factor:1 | 1 (-0.30392) | -1 | -1 |
| G: -6257.17264 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.95804 HOMO: -6.65318 LUMO: 0.04354 factor:1 | 1 (-0.41971) | -1 | -1 |
| G: -6257.17264 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.89110 HOMO: -6.94707 LUMO: -1.68438 factor:1 | 1 (-0.35277) | -1 | -1 |
| G: -6257.17264 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.32540 HOMO: -6.71849 LUMO: 0.15783 factor:1 | -1 (0.21293) | -1 | -1 |
| G: -6257.17264 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.33860 HOMO: -6.97156 LUMO: 0.43266 factor:1 | -1 (0.19973) | -1 | -1 |
| G: -6257.17264 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12520.95103 HOMO: -6.91441 LUMO: -0.54695 factor:1 | -1 (0.58730) | -1 | -1 |
| G: -6257.17264 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.20390 HOMO: -6.74842 LUMO: -0.76192 factor:1 | -1 (0.33443) | -1 | -1 |
| G: -6257.17264 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.66149 HOMO: -6.70489 LUMO: 0.19048 factor:1 | 1 (-0.12316) | -1 | -1 |
| G: -6257.17264 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.80655 HOMO: -7.25728 LUMO: 0.33470 factor:1 | 1 (-0.26822) | 1 | -1 |
| G: -6257.17264 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.70359 HOMO: -6.96339 LUMO: 0.55511 factor:1 | 1 (-0.16525) | -1 | -1 |
| G: -6257.17264 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12520.71211 HOMO: -6.77564 LUMO: 0.72382 factor:1 | -1 (0.82622) | -1 | -1 |
| G: -6257.17264 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12520.97443 HOMO: -6.75387 LUMO: 0.39729 factor:1 | -1 (0.56390) | -1 | -1 |
| G: -6257.17264 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.19811 HOMO: -7.00149 LUMO: 0.06531 factor:1 | -1 (0.34022) | -1 | -1 |
| G: -6257.17264 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12520.99636 HOMO: -7.09945 LUMO: 0.33470 factor:1 | -1 (0.54197) | 1 | 1 |
| G: -6257.17264 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.41661 HOMO: -7.20830 LUMO: 0.59593 factor:1 | -1 (0.12172) | 1 | 1 |
| G: -6257.17264 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.55313 HOMO: -6.40556 LUMO: 0.56600 factor:1 | 1 (-0.01480) | -1 | -1 |
| G: -6257.17264 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.53368 HOMO: -6.77291 LUMO: 0.73471 factor:1 | -1 (0.00465) | -1 | -1 |
| G: -6257.17264 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.49403 HOMO: -6.65046 LUMO: 0.09796 factor:1 | -1 (0.04430) | -1 | -1 |
| G: -6257.17264 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.02609 HOMO: -6.95795 LUMO: 0.22313 factor:1 | 1 (-0.48776) | -1 | -1 |
| G: -6257.17264 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.99331 HOMO: -6.85727 LUMO: 0.04626 factor:1 | 1 (-0.45497) | -1 | -1 |
| G: -6257.17264 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.91513 HOMO: -7.27360 LUMO: 0.42178 factor:1 | 1 (-0.37680) | 1 | 1 |
| G: -6257.17264 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.87646 HOMO: -6.78924 LUMO: -0.13334 factor:1 | 1 (-0.33813) | -1 | -1 |
| G: -6257.17264 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.96890 HOMO: -6.63141 LUMO: 0.38368 factor:1 | 1 (-0.43057) | -1 | -1 |
| G: -6257.17264 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.95948 HOMO: -6.92258 LUMO: 0.39184 factor:1 | 1 (-0.42115) | -1 | -1 |
| G: -6257.17264 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.82661 HOMO: -6.19331 LUMO: -0.46804 factor:1 | 1 (-0.28828) | -1 | -1 |
| G: -6257.17264 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.37893 HOMO: -7.26544 LUMO: -0.05442 factor:1 | -1 (0.15940) | 1 | 1 |
| G: -6257.17264 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.11280 HOMO: -7.09401 LUMO: 0.30749 factor:1 | -1 (0.42553) | 1 | 1 |
| G: -6257.17264 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.23784 HOMO: -6.14705 LUMO: -0.88709 factor:1 | -1 (0.30050) | -1 | -1 |
| G: -6257.17264 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.36646 HOMO: -6.53617 LUMO: -0.28572 factor:1 | -1 (0.17187) | -1 | -1 |
| G: -6257.17264 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.33119 HOMO: -6.37291 LUMO: -0.67212 factor:1 | 1 (-0.79286) | -1 | -1 |
| G: -6257.17264 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.36417 HOMO: -6.65591 LUMO: 0.03810 factor:1 | 1 (-0.82584) | -1 | -1 |
| G: -6257.17264 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.31282 HOMO: -7.11034 LUMO: 0.75103 factor:1 | 1 (-0.77449) | 1 | 1 |
| G: -6257.17264 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.57008 HOMO: -6.85183 LUMO: -0.05987 factor:1 | 1 (-1.03175) | -1 | -1 |
| G: -6257.17264 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.47103 HOMO: -6.70761 LUMO: -0.05442 factor:1 | 1 (-0.93270) | -1 | -1 |
| G: -6257.17264 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.55476 HOMO: -6.23413 LUMO: 0.06259 factor:1 | 1 (-1.01643) | -1 | -1 |
| G: -6257.17264 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.63914 HOMO: -6.55794 LUMO: 0.74015 factor:1 | 1 (-1.10081) | -1 | -1 |
| G: -6257.17264 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.37704 HOMO: -7.27905 LUMO: 0.26939 factor:1 | 1 (-0.83871) | 1 | 1 |
| G: -6257.17264 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.08550 HOMO: -6.34842 LUMO: -0.86804 factor:1 | 1 (-0.54717) | -1 | -1 |
| G: -6257.17264 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.04199 HOMO: -6.27222 LUMO: 1.46125 factor:1 | 1 (-0.50366) | -1 | -1 |
| G: -6257.17264 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.15048 HOMO: -6.65046 LUMO: 2.04902 factor:1 | 1 (-0.61215) | -1 | -1 |
| G: -6257.17264 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.82046 HOMO: -7.11850 LUMO: -1.14016 factor:1 | 1 (-0.28213) | 1 | -1 |
| G: -6257.17264 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.96307 HOMO: -6.88720 LUMO: -1.20274 factor:1 | 1 (-0.42474) | -1 | -1 |
| G: -6257.17264 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.06656 HOMO: -6.69400 LUMO: -0.31565 factor:1 | 1 (-0.52823) | -1 | -1 |
| G: -6257.17264 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.98599 HOMO: -6.95523 LUMO: -1.55377 factor:1 | 1 (-0.44765) | -1 | -1 |
| G: -6257.17264 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.81549 HOMO: -6.41372 LUMO: -0.83539 factor:1 | 1 (-2.27716) | -1 | -1 |
| G: -6257.17264 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.10105 HOMO: -6.13889 LUMO: -0.90070 factor:1 | 1 (-1.56272) | -1 | -1 |
| G: -6257.17264 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.81864 HOMO: -6.44366 LUMO: -0.55511 factor:1 | 1 (-2.28031) | -1 | -1 |
| G: -6257.17264 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.14171 HOMO: -6.10079 LUMO: -0.71022 factor:1 | 1 (-1.60338) | -1 | -1 |
| G: -6257.17264 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.10149 HOMO: -6.90353 LUMO: -0.64763 factor:1 | 1 (-1.56316) | -1 | -1 |
| G: -6257.17264 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.67225 HOMO: -6.65046 LUMO: -0.82450 factor:1 | 1 (-2.13392) | -1 | -1 |
| G: -6257.17264 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.23156 HOMO: -6.81645 LUMO: -0.85444 factor:1 | 1 (-1.69323) | -1 | -1 |
| G: -6257.17264 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.33581 HOMO: -6.20692 LUMO: 1.30887 factor:1 | 1 (-1.79748) | -1 | -1 |
| G: -6257.17264 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.61559 HOMO: -5.96201 LUMO: 1.33880 factor:1 | 1 (-2.07726) | -1 | -1 |
| G: -6257.17264 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.99361 HOMO: -6.52529 LUMO: 1.58914 factor:1 | 1 (-2.45528) | -1 | -1 |
| G: -6257.17264 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.12756 HOMO: -6.58516 LUMO: 1.97555 factor:1 | 1 (-1.58923) | -1 | -1 |
| G: -6257.17264 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.05330 HOMO: -6.84366 LUMO: 0.15783 factor:1 | 1 (-1.51497) | -1 | -1 |
| G: -6257.17264 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.46797 HOMO: -6.45726 LUMO: 0.42994 factor:1 | 1 (-1.92964) | -1 | -1 |
| G: -6257.17264 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.11371 HOMO: -6.75387 LUMO: 0.14422 factor:1 | 1 (-1.57538) | -1 | -1 |
| G: -6257.17264 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.67472 HOMO: -6.69944 LUMO: 1.79051 factor:1 | 1 (-2.13639) | -1 | -1 |
| G: -6257.17264 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.15637 HOMO: -6.59876 LUMO: 1.90208 factor:1 | 1 (-1.61804) | -1 | -1 |
| G: -6257.17264 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.18345 HOMO: -7.05863 LUMO: 1.20819 factor:1 | 1 (-1.64512) | -1 | -1 |
| G: -6257.17264 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.15624 HOMO: -6.54978 LUMO: 2.01636 factor:1 | 1 (-1.61791) | -1 | -1 |
| G: -6257.17264 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.96666 HOMO: -5.52119 LUMO: 1.95106 factor:1 | 1 (-1.42833) | -1 | -1 |
| G: -6257.17264 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.79786 HOMO: -6.53617 LUMO: 1.60275 factor:1 | 1 (-1.25953) | -1 | -1 |
| G: -6257.17264 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.06176 HOMO: -6.11440 LUMO: 1.89119 factor:1 | 1 (-1.52343) | -1 | -1 |
| G: -6257.17264 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.28400 HOMO: -7.31986 LUMO: 0.48708 factor:1 | 1 (-1.74566) | 1 | 1 |
| G: -6257.17264 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.24877 HOMO: -6.76475 LUMO: -0.75648 factor:1 | 1 (-0.71043) | -1 | -1 |
| G: -6257.17264 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.42425 HOMO: -6.76747 LUMO: -1.06941 factor:1 | 1 (-0.88592) | -1 | -1 |
| G: -6257.17264 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.85906 HOMO: -6.87087 LUMO: 0.72927 factor:1 | 1 (-1.32073) | -1 | -1 |
| G: -6257.17264 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.93019 HOMO: -7.00965 LUMO: 0.02177 factor:1 | 1 (-1.39186) | -1 | -1 |
| G: -6257.17264 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.93368 HOMO: -6.54706 LUMO: -0.03265 factor:1 | 1 (-1.39535) | -1 | -1 |
| G: -6257.17264 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.91686 HOMO: -6.62325 LUMO: -0.63675 factor:1 | 1 (-1.37853) | -1 | -1 |
| G: -6257.17264 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.55544 HOMO: -7.03414 LUMO: -1.24084 factor:1 | 1 (-1.01711) | -1 | -1 |
| G: -6257.17264 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.83925 HOMO: -7.04503 LUMO: -0.10068 factor:1 | 1 (-1.30092) | -1 | -1 |
| G: -6257.17264 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.86527 HOMO: -6.67223 LUMO: 0.03537 factor:1 | 1 (-1.32694) | -1 | -1 |
| G: -6257.17264 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.73601 HOMO: -6.82734 LUMO: 0.58777 factor:1 | 1 (-1.19768) | -1 | -1 |
| G: -6257.17264 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.34088 HOMO: -6.84366 LUMO: 0.46531 factor:1 | 1 (-0.80255) | -1 | -1 |
| G: -6257.17264 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.33318 HOMO: -7.03959 LUMO: -1.15104 factor:1 | 1 (-0.79484) | -1 | -1 |
| G: -6257.17264 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.16066 HOMO: -6.91169 LUMO: -0.41361 factor:1 | 1 (-0.62232) | -1 | -1 |
| G: -6257.17264 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.15519 HOMO: -7.10217 LUMO: -0.44627 factor:1 | 1 (-0.61685) | 1 | 1 |
| G: -6257.17264 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.31312 HOMO: -6.88176 LUMO: -0.19592 factor:1 | 1 (-0.77479) | -1 | -1 |
| G: -6257.17264 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.26166 HOMO: -7.21374 LUMO: -0.46531 factor:1 | 1 (-0.72333) | 1 | 1 |
| G: -6257.17264 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.08972 HOMO: -6.54978 LUMO: 0.16871 factor:1 | 1 (-0.55138) | -1 | -1 |
| G: -6257.17264 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.24419 HOMO: -6.71305 LUMO: -0.13061 factor:1 | 1 (-0.70586) | -1 | -1 |
| G: -6257.17264 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.38554 HOMO: -6.74842 LUMO: -0.36191 factor:1 | -1 (0.15279) | -1 | -1 |
| G: -6257.17264 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12520.93339 HOMO: -6.74570 LUMO: -0.09796 factor:1 | -1 (0.60494) | -1 | -1 |
| G: -6257.17264 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.09634 HOMO: -6.93890 LUMO: -0.27211 factor:1 | -1 (0.44199) | -1 | -1 |
| G: -6257.17264 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.11035 HOMO: -6.88720 LUMO: -0.18776 factor:1 | -1 (0.42798) | -1 | -1 |
| G: -6257.17264 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12520.98825 HOMO: -6.74842 LUMO: 0.02993 factor:1 | -1 (0.55008) | -1 | -1 |
| G: -6257.17264 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.13435 HOMO: -6.70216 LUMO: 0.01361 factor:1 | -1 (0.40398) | -1 | -1 |
| G: -6257.17264 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.30709 HOMO: -6.90625 LUMO: 0.00544 factor:1 | -1 (0.23124) | -1 | -1 |
| G: -6257.17264 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.08537 HOMO: -6.18243 LUMO: 0.25851 factor:1 | -1 (0.45296) | -1 | -1 |
| G: -6257.17264 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.42297 HOMO: -6.32937 LUMO: -0.20953 factor:1 | 1 (-0.88464) | -1 | -1 |
| G: -6257.17264 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.33984 HOMO: -6.78108 LUMO: 0.00544 factor:1 | 1 (-0.80151) | -1 | -1 |
| G: -6257.17264 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.11976 HOMO: -5.97562 LUMO: 0.28572 factor:1 | 1 (-0.58143) | -1 | -1 |
| G: -6257.17264 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12520.85617 HOMO: -5.97290 LUMO: -0.18504 factor:1 | -1 (0.68216) | -1 | -1 |
| G: -6257.17264 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.04330 HOMO: -6.12800 LUMO: 0.42178 factor:1 | -1 (0.49503) | -1 | -1 |
| G: -6257.17264 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.07617 HOMO: -6.24229 LUMO: -0.00816 factor:1 | -1 (0.46216) | -1 | -1 |
| G: -6257.17264 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.75152 HOMO: -6.61781 LUMO: 0.12789 factor:1 | 1 (-1.21319) | -1 | -1 |
| G: -6257.17264 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.53432 HOMO: -6.70489 LUMO: 0.14694 factor:1 | 1 (-0.99599) | -1 | -1 |
| G: -6257.17264 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.90451 HOMO: -6.86543 LUMO: -0.21225 factor:1 | 1 (-0.36618) | -1 | -1 |
| G: -6257.17264 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.72589 HOMO: -6.90081 LUMO: -0.20136 factor:1 | 1 (-1.18756) | -1 | -1 |
| G: -6257.17264 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.01573 HOMO: -7.12938 LUMO: -0.25851 factor:1 | 1 (-0.47740) | 1 | 1 |
| G: -6257.17264 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.05162 HOMO: -6.93074 LUMO: -0.26667 factor:1 | 1 (-0.51329) | -1 | -1 |
| G: -6257.17264 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.17366 HOMO: -7.00421 LUMO: -0.31021 factor:1 | 1 (-0.63533) | -1 | -1 |
| G: -6257.17264 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.03652 HOMO: -7.10761 LUMO: -0.17415 factor:1 | 1 (-0.49819) | 1 | 1 |
| G: -6257.17264 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.98569 HOMO: -8.21240 LUMO: 0.05987 factor:1 | 1 (-0.44736) | 1 | 1 |
| G: -6257.17264 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.02408 HOMO: -7.14843 LUMO: -0.46531 factor:1 | 1 (-0.48575) | 1 | -1 |
| G: -6257.17264 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.98286 HOMO: -6.80829 LUMO: -0.29933 factor:1 | 1 (-0.44453) | -1 | -1 |
| G: -6257.17264 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.94084 HOMO: -6.84094 LUMO: -0.53606 factor:1 | 1 (-0.40251) | -1 | -1 |
| G: -6257.17264 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.99809 HOMO: -6.81917 LUMO: -0.26667 factor:1 | 1 (-0.45976) | -1 | -1 |
| G: -6257.17264 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.48807 HOMO: -6.85727 LUMO: -1.20002 factor:1 | -1 (0.05026) | -1 | -1 |
| G: -6257.17264 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.99883 HOMO: -6.39468 LUMO: -1.06941 factor:1 | 1 (-0.46050) | -1 | -1 |
| G: -6257.17264 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.70652 HOMO: -6.00827 LUMO: -1.94017 factor:1 | 1 (-0.16819) | -1 | -1 |
| G: -6257.17264 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.96571 HOMO: -6.80829 LUMO: 0.18504 factor:1 | 1 (-0.42738) | -1 | -1 |
| G: -6257.17264 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.16569 HOMO: -6.54434 LUMO: -0.95784 factor:1 | 1 (-0.62736) | -1 | -1 |
| G: -6257.17264 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.57245 HOMO: -6.45454 LUMO: -0.07347 factor:1 | 1 (-0.03412) | -1 | -1 |
| G: -6257.17264 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.00691 HOMO: -5.33887 LUMO: 1.11839 factor:1 | 1 (-0.46858) | -1 | -1 |
| G: -6257.17264 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.05717 HOMO: -5.75249 LUMO: 0.70477 factor:1 | 1 (-0.51884) | -1 | -1 |
| G: -6257.17264 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.74489 HOMO: -5.64092 LUMO: 0.87076 factor:1 | 1 (-0.20656) | -1 | -1 |
| G: -6257.17264 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.02057 HOMO: -5.14295 LUMO: 1.06124 factor:1 | 1 (-0.48224) | -1 | -1 |
| G: -6257.17264 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.74764 HOMO: -5.05043 LUMO: 1.21091 factor:1 | 1 (-0.20931) | -1 | -1 |
| G: -6257.17264 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.79363 HOMO: -5.05588 LUMO: 1.02859 factor:1 | 1 (-0.25530) | -1 | -1 |
| G: -6257.17264 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.97203 HOMO: -5.76337 LUMO: 0.79457 factor:1 | 1 (-0.43370) | -1 | -1 |
| G: -6257.17264 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.36546 HOMO: -5.01506 LUMO: 1.00138 factor:1 | -1 (0.17287) | -1 | -1 |
| G: -6257.17264 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.02612 HOMO: -4.84363 LUMO: 1.53744 factor:1 | 1 (-0.48779) | -1 | -1 |
| G: -6257.17264 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.56636 HOMO: -5.17833 LUMO: 1.45309 factor:1 | 1 (-0.02803) | -1 | -1 |
| G: -6257.17264 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.94832 HOMO: -5.13751 LUMO: 0.51157 factor:1 | 1 (-0.40999) | -1 | -1 |
| G: -6257.17264 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.57482 HOMO: -5.56473 LUMO: 0.32109 factor:1 | 1 (-0.03649) | -1 | -1 |
| G: -6257.17264 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.77689 HOMO: -4.69941 LUMO: 1.14016 factor:1 | 1 (-0.23856) | -1 | -1 |
| G: -6257.17264 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.88808 HOMO: -4.49260 LUMO: 1.86398 factor:1 | 1 (-0.34975) | -1 | -1 |
| G: -6257.17264 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.91505 HOMO: -4.32117 LUMO: 1.68438 factor:1 | 1 (-0.37671) | -1 | -1 |
| G: -6257.17264 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.83306 HOMO: -4.44906 LUMO: 1.37690 factor:1 | 1 (-0.29473) | -1 | -1 |
| G: -6257.17264 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.94492 HOMO: -4.62049 LUMO: 1.34968 factor:1 | 1 (-0.40659) | -1 | -1 |
| G: -6257.17264 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.36115 HOMO: -4.59600 LUMO: 1.58370 factor:1 | 1 (-0.82282) | -1 | -1 |
| G: -6257.17264 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.31671 HOMO: -4.98785 LUMO: 1.46669 factor:1 | 1 (-0.77838) | -1 | -1 |
| G: -6257.17264 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.30262 HOMO: -5.06676 LUMO: 1.27349 factor:1 | 1 (-0.76429) | -1 | -1 |
| G: -6257.17264 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.40945 HOMO: -5.09125 LUMO: 1.13471 factor:1 | 1 (-0.87112) | -1 | -1 |
| G: -6257.17264 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.17018 HOMO: -4.84635 LUMO: 1.33608 factor:1 | 1 (-0.63185) | -1 | -1 |
| G: -6257.17264 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.85122 HOMO: -4.94431 LUMO: 1.18370 factor:1 | 1 (-2.31289) | -1 | -1 |
| G: -6257.17264 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12524.16431 HOMO: -4.92526 LUMO: 1.39867 factor:1 | 1 (-2.62598) | -1 | -1 |
| G: -6257.17264 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.62114 HOMO: -5.71983 LUMO: 0.60137 factor:1 | 1 (-2.08281) | -1 | -1 |
| G: -6257.17264 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.94599 HOMO: -5.10486 LUMO: 1.05580 factor:1 | 1 (-2.40766) | -1 | -1 |
| G: -6257.17264 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.17431 HOMO: -5.20282 LUMO: 1.01226 factor:1 | 1 (-1.63598) | -1 | -1 |
| G: -6257.17264 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.81530 HOMO: -4.98513 LUMO: 1.53744 factor:1 | 1 (-2.27697) | -1 | -1 |
| G: -6257.17264 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.52131 HOMO: -5.67085 LUMO: 0.17687 factor:1 | 1 (-1.98298) | -1 | -1 |
| G: -6257.17264 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.76513 HOMO: -5.87222 LUMO: 0.12517 factor:1 | 1 (-1.22680) | -1 | -1 |
| G: -6257.17264 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.22299 HOMO: -5.20826 LUMO: 0.91702 factor:1 | 1 (-1.68466) | -1 | -1 |
| G: -6257.17264 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.85802 HOMO: -5.94569 LUMO: 0.63130 factor:1 | 1 (-2.31969) | -1 | -1 |
| G: -6257.17264 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.68275 HOMO: -5.35792 LUMO: 0.91430 factor:1 | 1 (-2.14442) | -1 | -1 |
| G: -6257.17264 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.94641 HOMO: -5.36336 LUMO: 1.44220 factor:1 | 1 (-1.40808) | -1 | -1 |
| G: -6257.17264 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.53161 HOMO: -5.83412 LUMO: 0.71294 factor:1 | -1 (0.00672) | -1 | -1 |
| G: -6257.17264 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.94811 HOMO: -4.97696 LUMO: 1.72792 factor:1 | 1 (-0.40978) | -1 | -1 |
| G: -6257.17264 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.75099 HOMO: -5.55929 LUMO: 0.23130 factor:1 | 1 (-0.21266) | -1 | -1 |
| G: -6257.17264 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.88724 HOMO: -5.71167 LUMO: 0.47348 factor:1 | 1 (-0.34890) | -1 | -1 |
| G: -6257.17264 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.91850 HOMO: -7.31986 LUMO: -2.54699 factor:1 | 1 (-0.38017) | -1 | -1 |
| G: -6257.17264 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.78230 HOMO: -5.34704 LUMO: 1.19730 factor:1 | 1 (-1.24397) | -1 | -1 |
| G: -6257.17264 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.47867 HOMO: -5.45860 LUMO: 0.80818 factor:1 | 1 (-0.94034) | -1 | -1 |
| G: -6257.17264 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.47038 HOMO: -5.12663 LUMO: 1.20274 factor:1 | 1 (-0.93204) | -1 | -1 |
| G: -6257.17264 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.90641 HOMO: -5.37153 LUMO: 1.05580 factor:1 | 1 (-1.36808) | -1 | -1 |
| G: -6257.17264 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.66709 HOMO: -5.47221 LUMO: 0.97961 factor:1 | 1 (-1.12876) | -1 | -1 |
| G: -6257.17264 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.61171 HOMO: -5.06948 LUMO: 1.12111 factor:1 | 1 (-1.07338) | -1 | -1 |
| G: -6257.17264 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.79452 HOMO: -5.19737 LUMO: 1.25444 factor:1 | 1 (-1.25619) | -1 | -1 |
| G: -6257.17264 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.61153 HOMO: -5.27901 LUMO: 1.00682 factor:1 | 1 (-0.07320) | -1 | -1 |
| G: -6257.17264 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.67482 HOMO: -5.38513 LUMO: 0.49253 factor:1 | 1 (-0.13649) | -1 | -1 |
| G: -6257.17264 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.85953 HOMO: -5.12390 LUMO: 1.22995 factor:1 | 1 (-0.32120) | -1 | -1 |
| G: -6257.17264 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.01194 HOMO: -5.31438 LUMO: 0.70205 factor:1 | 1 (-0.47361) | -1 | -1 |
| G: -6257.17264 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.91330 HOMO: -5.17561 LUMO: 1.04492 factor:1 | 1 (-0.37497) | -1 | -1 |
| G: -6257.17264 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.65793 HOMO: -4.94431 LUMO: 1.52656 factor:1 | 1 (-2.11960) | -1 | -1 |
| G: -6257.17264 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.59562 HOMO: -5.13751 LUMO: 0.93879 factor:1 | 1 (-2.05729) | -1 | -1 |
| G: -6257.17264 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.03224 HOMO: -5.49942 LUMO: 0.97689 factor:1 | 1 (-1.49391) | -1 | -1 |
| G: -6257.17264 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.41910 HOMO: -5.79058 LUMO: 0.53879 factor:1 | 1 (-1.88077) | -1 | -1 |
| G: -6257.17264 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.70148 HOMO: -5.36881 LUMO: 1.56465 factor:1 | 1 (-1.16315) | -1 | -1 |
| G: -6257.17264 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.79781 HOMO: -4.67492 LUMO: 1.32792 factor:1 | 1 (-1.25948) | -1 | -1 |
| G: -6257.17264 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.94813 HOMO: -4.60145 LUMO: 1.19458 factor:1 | 1 (-1.40979) | -1 | -1 |
| G: -6257.17264 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.81092 HOMO: -4.49260 LUMO: 1.60547 factor:1 | 1 (-2.27259) | -1 | -1 |
| G: -6257.17264 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.06168 HOMO: -4.65043 LUMO: 1.34696 factor:1 | 1 (-1.52335) | -1 | -1 |
| G: -6257.17264 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.14097 HOMO: -4.77560 LUMO: 1.35241 factor:1 | 1 (-1.60264) | -1 | -1 |
| G: -6257.17264 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.10179 HOMO: -4.94431 LUMO: 1.17825 factor:1 | 1 (-1.56346) | -1 | -1 |
| G: -6257.17264 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.17042 HOMO: -4.87084 LUMO: 1.41771 factor:1 | 1 (-0.63209) | -1 | -1 |
| G: -6257.17264 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.13732 HOMO: -5.34432 LUMO: 1.16737 factor:1 | -1 (0.40101) | -1 | -1 |
| G: -6257.17264 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.50277 HOMO: -4.94975 LUMO: 1.67622 factor:1 | -1 (0.03557) | -1 | -1 |
| G: -6257.17264 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.52027 HOMO: -4.81369 LUMO: 1.14288 factor:1 | 1 (-1.98194) | -1 | -1 |
| G: -6257.17264 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.15556 HOMO: -5.22459 LUMO: 0.29660 factor:1 | 1 (-1.61723) | -1 | -1 |
| G: -6257.17264 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.35782 HOMO: -5.21642 LUMO: 0.37824 factor:1 | 1 (-1.81949) | -1 | -1 |
| G: -6257.17264 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12524.02450 HOMO: -5.00417 LUMO: 1.01226 factor:1 | 1 (-2.48617) | -1 | -1 |
| G: -6257.17264 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12524.15536 HOMO: -5.46677 LUMO: 0.10612 factor:1 | 1 (-2.61703) | -1 | -1 |
| G: -6257.17264 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.31681 HOMO: -5.51303 LUMO: 0.54151 factor:1 | 1 (-1.77848) | -1 | -1 |
| G: -6257.17264 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.37877 HOMO: -5.63004 LUMO: 0.17960 factor:1 | 1 (-1.84044) | -1 | -1 |
| G: -6257.17264 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12524.07528 HOMO: -4.79193 LUMO: 1.12111 factor:1 | 1 (-2.53694) | -1 | -1 |
| G: -6257.17264 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.98181 HOMO: -5.43411 LUMO: 0.45987 factor:1 | 1 (-1.44348) | -1 | -1 |
| G: -6257.17264 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.45835 HOMO: -7.06135 LUMO: -2.13881 factor:1 | 1 (-0.92002) | 1 | 1 |
| G: -6257.17264 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.15839 HOMO: -5.33071 LUMO: 1.14016 factor:1 | 1 (-1.62006) | -1 | -1 |
| G: -6257.17264 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.27725 HOMO: -7.12394 LUMO: -0.03810 factor:1 | 1 (-1.73892) | 1 | 1 |
| G: -6257.17264 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.08313 HOMO: -7.20558 LUMO: -2.50889 factor:1 | 1 (-0.54480) | 1 | 1 |
| G: -6257.17264 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.14830 HOMO: -7.26816 LUMO: -2.11432 factor:1 | 1 (-0.60997) | 1 | 1 |
| G: -6257.17264 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.52787 HOMO: -7.89674 LUMO: 0.31021 factor:1 | 1 (-0.98954) | 1 | 1 |
| G: -6257.17264 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.39146 HOMO: -7.26544 LUMO: 0.22858 factor:1 | 1 (-0.85313) | 1 | 1 |
| G: -6257.17264 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.34571 HOMO: -7.12666 LUMO: -0.02449 factor:1 | 1 (-1.80738) | 1 | 1 |
| G: -6257.17264 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.16693 HOMO: -7.68722 LUMO: 0.71838 factor:1 | 1 (-1.62860) | 1 | 1 |
| G: -6257.17264 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.21494 HOMO: -6.86271 LUMO: -0.96056 factor:1 | 1 (-0.67661) | -1 | -1 |
| G: -6257.17264 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.09570 HOMO: -7.07496 LUMO: -1.11839 factor:1 | 1 (-0.55737) | 1 | 1 |
| G: -6257.17264 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.59313 HOMO: -7.06952 LUMO: -2.08439 factor:1 | 1 (-1.05479) | 1 | 1 |
| G: -6257.17264 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.99498 HOMO: -6.60965 LUMO: -2.11977 factor:1 | 1 (-1.45665) | -1 | -1 |
| G: -6257.17264 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.00913 HOMO: -6.87360 LUMO: -1.85854 factor:1 | 1 (-1.47080) | -1 | -1 |
| G: -6257.17264 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.96471 HOMO: -7.67089 LUMO: -0.24762 factor:1 | 1 (-0.42638) | 1 | 1 |
| G: -6257.17264 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.94299 HOMO: -6.45726 LUMO: -1.86398 factor:1 | 1 (-0.40466) | -1 | -1 |
| G: -6257.17264 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.22400 HOMO: -6.91713 LUMO: 0.33198 factor:1 | 1 (-0.68567) | -1 | -1 |
| G: -6257.17264 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.21015 HOMO: -6.83278 LUMO: 0.26667 factor:1 | 1 (-0.67182) | -1 | -1 |
| G: -6257.17264 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.64408 HOMO: -6.89264 LUMO: -1.00682 factor:1 | 1 (-2.10575) | -1 | -1 |
| G: -6257.17264 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12524.37887 HOMO: -6.57427 LUMO: 0.22041 factor:1 | 1 (-2.84054) | -1 | -1 |
| G: -6257.17264 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.28065 HOMO: -7.52123 LUMO: -0.01905 factor:1 | 1 (-1.74232) | 1 | 1 |
| G: -6257.17264 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.07556 HOMO: -7.37429 LUMO: -0.08980 factor:1 | 1 (-1.53723) | 1 | 1 |
| G: -6257.17264 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.95107 HOMO: -7.28449 LUMO: -0.26395 factor:1 | 1 (-0.41274) | 1 | 1 |
| G: -6257.17264 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.58526 HOMO: -6.79740 LUMO: -0.60954 factor:1 | 1 (-1.04693) | -1 | -1 |
| G: -6257.17264 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.30224 HOMO: -7.12666 LUMO: -0.60681 factor:1 | 1 (-0.76391) | 1 | 1 |
| G: -6257.17264 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.97409 HOMO: -6.96611 LUMO: -0.30477 factor:1 | 1 (-1.43575) | -1 | -1 |
| G: -6257.17264 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.82273 HOMO: -7.08040 LUMO: -0.31293 factor:1 | 1 (-2.28440) | 1 | 1 |
| G: -6257.17264 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12524.02009 HOMO: -6.78924 LUMO: -0.73743 factor:1 | 1 (-2.48176) | -1 | -1 |
| G: -6257.17264 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12524.11304 HOMO: -7.57293 LUMO: -1.11295 factor:1 | 1 (-2.57471) | 1 | 1 |
| G: -6257.17264 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.06726 HOMO: -7.15932 LUMO: -0.23130 factor:1 | 1 (-1.52893) | 1 | 1 |
| G: -6257.17264 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.33668 HOMO: -7.48585 LUMO: -0.10068 factor:1 | 1 (-1.79835) | 1 | 1 |
| G: -6257.17264 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.02990 HOMO: -7.17020 LUMO: -0.26123 factor:1 | 1 (-1.49156) | 1 | 1 |
| G: -6257.17264 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.25020 HOMO: -7.43143 LUMO: -0.16055 factor:1 | 1 (-1.71187) | 1 | 1 |
| G: -6257.17264 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.88233 HOMO: -7.14843 LUMO: -0.10612 factor:1 | 1 (-1.34400) | 1 | 1 |
| G: -6257.17264 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.80674 HOMO: -6.95523 LUMO: -0.22585 factor:1 | 1 (-1.26840) | -1 | -1 |
| G: -6257.17264 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.04570 HOMO: -7.06680 LUMO: -0.51974 factor:1 | -1 (0.49263) | 1 | 1 |
| G: -6257.17264 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.18121 HOMO: -6.80829 LUMO: -0.64763 factor:1 | -1 (0.35712) | -1 | -1 |
| G: -6257.17264 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.05454 HOMO: -7.13210 LUMO: -0.48164 factor:1 | -1 (0.48379) | 1 | 1 |
| G: -6257.17264 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.30140 HOMO: -7.16204 LUMO: -0.45715 factor:1 | -1 (0.23693) | 1 | 1 |
| G: -6257.17264 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.03896 HOMO: -7.15115 LUMO: -0.43266 factor:1 | 1 (-1.50063) | 1 | 1 |
| G: -6257.17264 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.23322 HOMO: -7.15932 LUMO: -2.52794 factor:1 | 1 (-1.69489) | -1 | -1 |
| G: -6257.17264 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.92611 HOMO: -7.21102 LUMO: -2.65311 factor:1 | 1 (-1.38778) | -1 | -1 |
| G: -6257.17264 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.88059 HOMO: -6.57427 LUMO: -2.78645 factor:1 | 1 (-1.34226) | -1 | -1 |
| G: -6257.17264 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.01141 HOMO: -6.40828 LUMO: -3.23815 factor:1 | -1 (0.52692) | -1 | -1 |
| G: -6257.17264 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.15441 HOMO: -7.71987 LUMO: -0.20953 factor:1 | -1 (0.38393) | 1 | 1 |
| G: -6257.17264 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.27186 HOMO: -7.47769 LUMO: -0.43810 factor:1 | 1 (-1.73353) | 1 | 1 |
| G: -6257.17264 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.21145 HOMO: -6.68040 LUMO: -2.22589 factor:1 | 1 (-1.67312) | -1 | -1 |
| G: -6257.17264 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.11469 HOMO: -6.92802 LUMO: -1.99187 factor:1 | 1 (-1.57636) | -1 | -1 |
| G: -6257.17264 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.83855 HOMO: -7.73620 LUMO: 0.01633 factor:1 | 1 (-0.30022) | 1 | 1 |
| G: -6257.17264 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.70889 HOMO: -7.28721 LUMO: -0.18504 factor:1 | 1 (-0.17056) | 1 | 1 |
| G: -6257.17264 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.89654 HOMO: -7.49674 LUMO: -0.19864 factor:1 | 1 (-0.35821) | 1 | 1 |
| G: -6257.17264 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.57785 HOMO: -7.10489 LUMO: -2.56331 factor:1 | 1 (-2.03952) | -1 | -1 |
| G: -6257.17264 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.90206 HOMO: -7.36612 LUMO: 0.16055 factor:1 | 1 (-1.36373) | 1 | 1 |
| G: -6257.17264 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.75936 HOMO: -7.67633 LUMO: 0.33198 factor:1 | 1 (-1.22103) | 1 | 1 |
| G: -6257.17264 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.89466 HOMO: -7.07768 LUMO: -0.27483 factor:1 | 1 (-1.35632) | 1 | 1 |
| G: -6257.17264 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12520.10557 HOMO: -7.32531 LUMO: 0.05442 factor:1 | -1 (1.43276) | 1 | 1 |
| G: -6257.17264 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12520.36568 HOMO: -6.79740 LUMO: -1.21635 factor:1 | -1 (1.17265) | -1 | -1 |
| G: -6257.17264 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12520.64373 HOMO: -7.14027 LUMO: 0.12517 factor:1 | -1 (0.89460) | 1 | -1 |
| G: -6257.17264 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12520.79271 HOMO: -7.17292 LUMO: 0.16871 factor:1 | -1 (0.74562) | 1 | -1 |
| G: -6257.17264 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.46887 HOMO: -7.08312 LUMO: -1.38778 factor:1 | 1 (-1.93054) | 1 | 1 |
| G: -6257.17264 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.25186 HOMO: -6.75387 LUMO: -1.88031 factor:1 | 1 (-1.71353) | -1 | -1 |
| G: -6257.17264 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.49655 HOMO: -7.07768 LUMO: -1.25717 factor:1 | 1 (-0.95822) | 1 | 1 |
| G: -6257.17264 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.72434 HOMO: -6.46543 LUMO: -1.14016 factor:1 | 1 (-1.18601) | -1 | -1 |
| G: -6257.17264 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.17061 HOMO: -7.37973 LUMO: -0.45987 factor:1 | 1 (-0.63228) | 1 | 1 |
| G: -6257.17264 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.99692 HOMO: -7.46408 LUMO: 0.03265 factor:1 | 1 (-0.45859) | 1 | 1 |
| G: -6257.17264 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.05535 HOMO: -7.96477 LUMO: -0.19864 factor:1 | 1 (-0.51702) | 1 | 1 |
| G: -6257.17264 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.18830 HOMO: -6.93890 LUMO: -1.11839 factor:1 | 1 (-0.64997) | -1 | -1 |
| G: -6257.17264 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12520.99957 HOMO: -7.06408 LUMO: -1.08846 factor:1 | -1 (0.53876) | 1 | 1 |
| G: -6257.17264 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.26975 HOMO: -7.14027 LUMO: -0.33470 factor:1 | -1 (0.26858) | 1 | 1 |
| G: -6257.17264 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.23088 HOMO: -7.38245 LUMO: 0.10885 factor:1 | 1 (-1.69255) | 1 | 1 |
| G: -6257.17264 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.46009 HOMO: -7.59470 LUMO: -1.21363 factor:1 | 1 (-0.92176) | 1 | 1 |
| G: -6257.17264 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.33630 HOMO: -7.23279 LUMO: -1.23812 factor:1 | 1 (-1.79797) | 1 | 1 |
| G: -6257.17264 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.18535 HOMO: -6.90897 LUMO: 0.23402 factor:1 | 1 (-1.64702) | -1 | -1 |
| G: -6257.17264 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.00753 HOMO: -7.36340 LUMO: -0.17143 factor:1 | 1 (-1.46920) | 1 | 1 |
| G: -6257.17264 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.23905 HOMO: -6.61781 LUMO: -0.01361 factor:1 | 1 (-0.70072) | -1 | -1 |
| G: -6257.17264 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.37549 HOMO: -6.80013 LUMO: 0.38368 factor:1 | 1 (-0.83716) | -1 | -1 |
| G: -6257.17264 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.57008 HOMO: -6.72121 LUMO: -0.95512 factor:1 | 1 (-1.03175) | -1 | -1 |
| G: -6257.17264 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.42923 HOMO: -6.24773 LUMO: -0.69933 factor:1 | 1 (-0.89090) | -1 | -1 |
| G: -6257.17264 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.17105 HOMO: -6.56883 LUMO: 0.14694 factor:1 | 1 (-0.63272) | -1 | -1 |
| G: -6257.17264 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12520.83919 HOMO: -6.51441 LUMO: -1.27621 factor:1 | -1 (0.69914) | -1 | -1 |
| G: -6257.17264 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.02872 HOMO: -6.91986 LUMO: -1.16737 factor:1 | -1 (0.50961) | -1 | -1 |
| G: -6257.17264 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.31766 HOMO: -6.17971 LUMO: -0.65307 factor:1 | 1 (-0.77933) | -1 | -1 |
| G: -6257.17264 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.14944 HOMO: -7.22462 LUMO: 0.04354 factor:1 | 1 (-0.61111) | 1 | 1 |
| G: -6257.17264 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.03649 HOMO: -7.16204 LUMO: -0.23674 factor:1 | 1 (-0.49816) | 1 | 1 |
| G: -6257.17264 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.99426 HOMO: -6.81645 LUMO: -0.19320 factor:1 | 1 (-0.45593) | -1 | -1 |
| G: -6257.17264 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.20757 HOMO: -6.69400 LUMO: 0.04082 factor:1 | 1 (-0.66924) | -1 | -1 |
| G: -6257.17264 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.45184 HOMO: -6.63141 LUMO: -0.22858 factor:1 | 1 (-0.91351) | -1 | -1 |
| G: -6257.17264 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.86383 HOMO: -6.92258 LUMO: -1.11295 factor:1 | 1 (-0.32550) | -1 | -1 |
| G: -6257.17264 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.62641 HOMO: -6.60148 LUMO: -1.13744 factor:1 | 1 (-1.08807) | -1 | -1 |
| G: -6257.17264 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.04136 HOMO: -6.78108 LUMO: -0.82450 factor:1 | 1 (-0.50303) | -1 | -1 |
| G: -6257.17264 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.89396 HOMO: -7.05591 LUMO: -0.97145 factor:1 | 1 (-0.35563) | -1 | -1 |
| G: -6257.17264 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.87956 HOMO: -6.65318 LUMO: -1.26261 factor:1 | 1 (-0.34123) | -1 | -1 |
| G: -6257.17264 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.74685 HOMO: -6.98244 LUMO: -0.98233 factor:1 | 1 (-0.20852) | -1 | -1 |
| G: -6257.17264 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.11048 HOMO: -7.11850 LUMO: -0.99594 factor:1 | 1 (-0.57215) | 1 | 1 |
| G: -6257.17264 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.92008 HOMO: -6.64230 LUMO: -0.93879 factor:1 | 1 (-0.38175) | -1 | -1 |
| G: -6257.17264 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12520.29246 HOMO: -6.62053 LUMO: -1.22451 factor:1 | -1 (1.24587) | -1 | -1 |
| G: -6257.17264 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12520.59088 HOMO: -7.02598 LUMO: -0.85172 factor:1 | -1 (0.94745) | -1 | -1 |
| G: -6257.17264 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12520.75350 HOMO: -7.06680 LUMO: -0.89253 factor:1 | -1 (0.78483) | 1 | 1 |
| G: -6257.17264 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.05816 HOMO: -7.17292 LUMO: 0.00272 factor:1 | -1 (0.48017) | 1 | 1 |
| G: -6257.17264 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.08387 HOMO: -7.03142 LUMO: -0.35103 factor:1 | -1 (0.45446) | -1 | -1 |
| G: -6257.17264 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.34791 HOMO: -6.96884 LUMO: -0.09796 factor:1 | -1 (0.19043) | -1 | -1 |
| G: -6257.17264 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.09821 HOMO: -6.56339 LUMO: -0.99322 factor:1 | -1 (0.44012) | -1 | -1 |
| G: -6257.17264 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.37014 HOMO: -7.08857 LUMO: -0.17687 factor:1 | -1 (0.16819) | 1 | 1 |
| G: -6257.17264 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.44614 HOMO: -7.05863 LUMO: -0.22041 factor:1 | -1 (0.09219) | -1 | -1 |
| G: -6257.17264 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.67820 HOMO: -7.15115 LUMO: -0.17960 factor:1 | 1 (-0.13987) | 1 | 1 |
| G: -6257.17264 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.69325 HOMO: -6.67495 LUMO: -0.96600 factor:1 | 1 (-0.15491) | -1 | -1 |
| G: -6257.17264 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.92819 HOMO: -6.74026 LUMO: -1.79867 factor:1 | 1 (-0.38986) | -1 | -1 |
| G: -6257.17264 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12520.80697 HOMO: -6.73482 LUMO: -1.78235 factor:1 | -1 (0.73136) | -1 | -1 |
| G: -6257.17264 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12520.70365 HOMO: -6.09807 LUMO: 0.16871 factor:1 | -1 (0.83468) | -1 | -1 |
| G: -6257.17264 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12520.75872 HOMO: -6.72393 LUMO: 0.27211 factor:1 | -1 (0.77961) | -1 | -1 |
| G: -6257.17264 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12520.91021 HOMO: -6.40556 LUMO: -0.04354 factor:1 | -1 (0.62812) | -1 | -1 |
| G: -6257.17264 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.02940 HOMO: -6.56883 LUMO: 0.22041 factor:1 | -1 (0.50893) | -1 | -1 |
| G: -6257.17264 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12520.89122 HOMO: -7.22462 LUMO: 0.15783 factor:1 | -1 (0.64711) | 1 | 1 |
| G: -6257.17264 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.12426 HOMO: -6.83550 LUMO: 0.19320 factor:1 | -1 (0.41408) | -1 | -1 |
| G: -6257.17264 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.97352 HOMO: -7.26816 LUMO: -0.07619 factor:1 | 1 (-0.43519) | 1 | -1 |
| G: -6257.17264 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.86049 HOMO: -7.13483 LUMO: 0.33198 factor:1 | 1 (-0.32216) | 1 | 1 |
| G: -6257.17264 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.10727 HOMO: -6.58243 LUMO: -0.26395 factor:1 | 1 (-0.56894) | -1 | -1 |
| G: -6257.17264 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.37491 HOMO: -7.38517 LUMO: 0.17143 factor:1 | 1 (-1.83658) | 1 | 1 |
| G: -6257.17264 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.27629 HOMO: -6.80013 LUMO: 0.25851 factor:1 | 1 (-1.73796) | -1 | -1 |
| G: -6257.17264 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.42344 HOMO: -6.96611 LUMO: 0.11429 factor:1 | 1 (-0.88510) | -1 | -1 |
| G: -6257.17264 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.08786 HOMO: -6.51713 LUMO: -1.14560 factor:1 | 1 (-1.54953) | -1 | -1 |
| G: -6257.17264 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.24036 HOMO: -7.15387 LUMO: -0.35647 factor:1 | 1 (-0.70203) | 1 | 1 |
| G: -6257.17264 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.50534 HOMO: -5.26540 LUMO: 1.26805 factor:1 | 1 (-0.96701) | -1 | -1 |
| G: -6257.17264 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12520.14429 HOMO: -6.76475 LUMO: -0.16327 factor:1 | -1 (1.39404) | -1 | -1 |
| G: -6257.17264 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12520.01264 HOMO: -6.55250 LUMO: -0.71838 factor:1 | -1 (1.52569) | -1 | -1 |
| G: -6257.17264 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12520.21159 HOMO: -6.76203 LUMO: -1.08301 factor:1 | -1 (1.32675) | -1 | -1 |
| G: -6257.17264 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.13277 HOMO: -7.14027 LUMO: -0.01633 factor:1 | -1 (0.40556) | 1 | 1 |
| G: -6257.17264 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12520.95255 HOMO: -6.94979 LUMO: -0.93879 factor:1 | -1 (0.58578) | -1 | -1 |
| G: -6257.17264 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.16126 HOMO: -6.74842 LUMO: 0.31293 factor:1 | -1 (0.37707) | -1 | -1 |
| G: -6257.17264 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12520.80066 HOMO: -6.43821 LUMO: 0.05987 factor:1 | -1 (0.73767) | -1 | -1 |
| G: -6257.17264 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12520.61755 HOMO: -6.60420 LUMO: 0.22585 factor:1 | -1 (0.92078) | -1 | -1 |
| G: -6257.17264 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12520.84907 HOMO: -6.43821 LUMO: 0.05987 factor:1 | -1 (0.68926) | -1 | -1 |
| G: -6257.17264 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.39076 HOMO: -6.34570 LUMO: 1.43948 factor:1 | -1 (0.14757) | -1 | -1 |
| G: -6257.17264 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.32137 HOMO: -6.03004 LUMO: 1.21363 factor:1 | -1 (0.21696) | -1 | -1 |
| G: -6257.17264 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.55460 HOMO: -6.68040 LUMO: -0.92247 factor:1 | 1 (-0.01627) | -1 | -1 |
| G: -6257.17264 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.36911 HOMO: -6.92530 LUMO: -0.31293 factor:1 | 1 (-1.83078) | -1 | -1 |
| G: -6257.17264 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.38422 HOMO: -6.94979 LUMO: -0.19864 factor:1 | 1 (-1.84588) | -1 | -1 |
| G: -6257.17264 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.45623 HOMO: -6.80829 LUMO: -0.30477 factor:1 | 1 (-0.91789) | -1 | -1 |
| G: -6257.17264 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.27794 HOMO: -7.22734 LUMO: -1.02859 factor:1 | 1 (-0.73961) | 1 | 1 |
| G: -6257.17264 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.09567 HOMO: -6.93890 LUMO: -0.72382 factor:1 | 1 (-1.55733) | -1 | -1 |
| G: -6257.17264 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.45756 HOMO: -7.27088 LUMO: -0.78097 factor:1 | 1 (-0.91923) | 1 | 1 |
| G: -6257.17264 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.53059 HOMO: -7.29809 LUMO: -0.97145 factor:1 | 1 (-0.99226) | 1 | 1 |
| G: -6257.17264 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.38134 HOMO: -7.18925 LUMO: -0.94696 factor:1 | 1 (-0.84301) | 1 | 1 |
| G: -6257.17264 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.28365 HOMO: -7.33891 LUMO: -0.96873 factor:1 | 1 (-0.74532) | 1 | 1 |
| G: -6257.17264 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.25554 HOMO: -7.36068 LUMO: -0.28028 factor:1 | 1 (-0.71721) | 1 | 1 |
| G: -6257.17264 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.50651 HOMO: -7.10761 LUMO: -1.14832 factor:1 | 1 (-0.96818) | 1 | 1 |
| G: -6257.17264 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.90781 HOMO: -6.94707 LUMO: -0.65307 factor:1 | 1 (-0.36948) | -1 | -1 |
| G: -6257.17264 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.15015 HOMO: -6.91713 LUMO: -1.81228 factor:1 | 1 (-0.61182) | -1 | -1 |
| G: -6257.17264 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.33560 HOMO: -6.78652 LUMO: -2.01636 factor:1 | 1 (-0.79727) | -1 | -1 |
| G: -6257.17264 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.22896 HOMO: -6.52801 LUMO: -1.17553 factor:1 | 1 (-0.69062) | -1 | -1 |
| G: -6257.17264 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.03801 HOMO: -7.54844 LUMO: -1.18642 factor:1 | 1 (-0.49968) | 1 | -1 |
| G: -6257.17264 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.05872 HOMO: -7.52939 LUMO: -1.23812 factor:1 | 1 (-0.52039) | 1 | -1 |
| G: -6257.17264 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.27976 HOMO: -7.94572 LUMO: -0.81634 factor:1 | 1 (-0.74143) | 1 | 1 |
| G: -6257.17264 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12520.86379 HOMO: -7.55932 LUMO: -0.86260 factor:1 | -1 (0.67454) | 1 | 1 |
| G: -6257.17264 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.14265 HOMO: -7.72259 LUMO: -1.39050 factor:1 | -1 (0.39568) | 1 | -1 |
| G: -6257.17264 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.38501 HOMO: -7.11850 LUMO: -1.01498 factor:1 | 1 (-0.84668) | 1 | -1 |
| G: -6257.17264 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.10787 HOMO: -7.09673 LUMO: -1.00954 factor:1 | 1 (-0.56953) | 1 | -1 |
| G: -6257.17264 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12520.81818 HOMO: -6.06270 LUMO: 0.16327 factor:1 | -1 (0.72015) | -1 | -1 |
| G: -6257.17264 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.07549 HOMO: -5.71167 LUMO: 0.70477 factor:1 | -1 (0.46284) | -1 | -1 |
| G: -6257.17264 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.40327 HOMO: -5.38241 LUMO: 0.86260 factor:1 | 1 (-0.86494) | -1 | -1 |
| G: -6257.17264 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.32507 HOMO: -5.67357 LUMO: 1.27621 factor:1 | 1 (-0.78674) | -1 | -1 |
| G: -6257.17264 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.81493 HOMO: -7.56204 LUMO: -0.68573 factor:1 | 1 (-0.27660) | 1 | 1 |
| G: -6257.17264 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.53266 HOMO: -5.57833 LUMO: 1.13199 factor:1 | 1 (-0.99433) | -1 | -1 |
| G: -6257.17264 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.08729 HOMO: -7.58653 LUMO: -0.66124 factor:1 | 1 (-0.54896) | 1 | 1 |
| G: -6257.17264 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12520.66033 HOMO: -7.91851 LUMO: -1.10206 factor:1 | -1 (0.87800) | 1 | -1 |
| G: -6257.17264 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12520.91783 HOMO: -6.48992 LUMO: -1.00138 factor:1 | -1 (0.62050) | -1 | -1 |
| G: -6257.17264 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12520.73048 HOMO: -7.09673 LUMO: -0.45171 factor:1 | -1 (0.80785) | 1 | 1 |
| G: -6257.17264 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12520.97043 HOMO: -6.63686 LUMO: 0.09252 factor:1 | -1 (0.56790) | -1 | -1 |
| G: -6257.17264 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.46992 HOMO: -6.84366 LUMO: -0.14422 factor:1 | -1 (0.06841) | -1 | -1 |
| G: -6257.17264 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.75706 HOMO: -6.93074 LUMO: 0.04354 factor:1 | 1 (-0.21873) | -1 | -1 |
| G: -6257.17264 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12520.84675 HOMO: -6.90353 LUMO: -0.19864 factor:1 | -1 (0.69158) | -1 | -1 |
| G: -6257.17264 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.10099 HOMO: -6.59876 LUMO: -0.10068 factor:1 | -1 (0.43734) | -1 | -1 |
| G: -6257.17264 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12524.34127 HOMO: -6.74570 LUMO: -0.44627 factor:1 | 1 (-2.80294) | -1 | -1 |
| G: -6257.17264 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.98145 HOMO: -6.60148 LUMO: -0.61770 factor:1 | 1 (-2.44312) | -1 | -1 |
| G: -6257.17264 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.31891 HOMO: -6.55794 LUMO: -1.06941 factor:1 | 1 (-1.78058) | -1 | -1 |
| G: -6257.17264 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12524.14771 HOMO: -7.12666 LUMO: -0.11973 factor:1 | 1 (-2.60938) | 1 | 1 |
| G: -6257.17264 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.76460 HOMO: -7.21646 LUMO: -0.50069 factor:1 | 1 (-2.22627) | 1 | 1 |
| G: -6257.17264 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.81716 HOMO: -7.27632 LUMO: -1.00682 factor:1 | 1 (-1.27883) | 1 | -1 |
| G: -6257.17264 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.68678 HOMO: -6.74298 LUMO: 0.04354 factor:1 | 1 (-2.14845) | -1 | -1 |
| G: -6257.17264 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.61774 HOMO: -6.37291 LUMO: 0.14150 factor:1 | 1 (-2.07941) | -1 | -1 |
| G: -6257.17264 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.02971 HOMO: -5.61371 LUMO: 1.28438 factor:1 | 1 (-1.49137) | -1 | -1 |
| G: -6257.17264 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.90327 HOMO: -5.52119 LUMO: 0.99866 factor:1 | 1 (-2.36494) | -1 | -1 |
| G: -6257.17264 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.77100 HOMO: -6.51985 LUMO: -0.10885 factor:1 | 1 (-2.23267) | -1 | -1 |
| G: -6257.17264 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12520.88629 HOMO: -5.61371 LUMO: 0.77280 factor:1 | -1 (0.65204) | -1 | -1 |
| G: -6257.17264 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.13128 HOMO: -5.58922 LUMO: 0.24490 factor:1 | -1 (0.40706) | -1 | -1 |
| G: -6257.17264 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.98792 HOMO: -6.32665 LUMO: -0.57144 factor:1 | 1 (-0.44959) | -1 | -1 |
| G: -6257.17264 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.78190 HOMO: -6.29127 LUMO: -0.93607 factor:1 | 1 (-0.24357) | -1 | -1 |
| G: -6257.17264 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.75093 HOMO: -5.49670 LUMO: 0.27211 factor:1 | 1 (-0.21260) | -1 | -1 |
| G: -6257.17264 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.88136 HOMO: -5.68990 LUMO: 0.24218 factor:1 | 1 (-0.34303) | -1 | -1 |
| G: -6257.17264 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.01156 HOMO: -5.68174 LUMO: 0.69933 factor:1 | 1 (-0.47323) | -1 | -1 |
| G: -6257.17264 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.94299 HOMO: -5.28173 LUMO: 1.00954 factor:1 | 1 (-0.40466) | -1 | -1 |
| G: -6257.17264 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.67063 HOMO: -5.94025 LUMO: 0.73471 factor:1 | 1 (-0.13230) | -1 | -1 |
| G: -6257.17264 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.89306 HOMO: -5.65725 LUMO: 1.28710 factor:1 | 1 (-0.35473) | -1 | -1 |
| G: -6257.17264 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.84828 HOMO: -5.41507 LUMO: 0.87076 factor:1 | 1 (-2.30995) | -1 | -1 |
| G: -6257.17264 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.68161 HOMO: -5.96474 LUMO: 0.29660 factor:1 | 1 (-2.14328) | -1 | -1 |
| G: -6257.17264 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.79746 HOMO: -7.00421 LUMO: 0.08708 factor:1 | 1 (-1.25913) | -1 | -1 |
| G: -6257.17264 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.15145 HOMO: -5.40418 LUMO: 0.90070 factor:1 | 1 (-1.61312) | -1 | -1 |
| G: -6257.17264 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.52256 HOMO: -7.00421 LUMO: -0.30477 factor:1 | 1 (-1.98423) | -1 | -1 |
| G: -6257.17264 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.76129 HOMO: -5.85861 LUMO: 0.74015 factor:1 | 1 (-1.22296) | -1 | -1 |
| G: -6257.17264 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.77384 HOMO: -5.71439 LUMO: 0.26395 factor:1 | 1 (-1.23551) | -1 | -1 |
| G: -6257.17264 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.81040 HOMO: -7.13755 LUMO: -0.78369 factor:1 | 1 (-2.27207) | 1 | -1 |
| G: -6257.17264 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.94413 HOMO: -7.31442 LUMO: -0.98233 factor:1 | 1 (-1.40579) | 1 | -1 |
| G: -6257.17264 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.03934 HOMO: -7.25728 LUMO: -1.00410 factor:1 | 1 (-1.50101) | 1 | -1 |
| G: -6257.17264 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.51037 HOMO: -7.48585 LUMO: -0.83811 factor:1 | 1 (-1.97204) | 1 | -1 |
| G: -6257.17264 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12524.12788 HOMO: -7.24911 LUMO: -0.77280 factor:1 | 1 (-2.58954) | 1 | -1 |
| G: -6257.17264 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.28857 HOMO: -7.55116 LUMO: -1.19730 factor:1 | 1 (-1.75024) | 1 | -1 |
| G: -6257.17264 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.30386 HOMO: -5.76881 LUMO: 0.28028 factor:1 | 1 (-1.76553) | -1 | -1 |
| G: -6257.17264 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.96102 HOMO: -5.77153 LUMO: -0.26939 factor:1 | 1 (-1.42269) | -1 | -1 |
| G: -6257.17264 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.00833 HOMO: -5.82868 LUMO: 0.36735 factor:1 | 1 (-0.47000) | -1 | -1 |
| G: -6257.17264 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.97325 HOMO: -5.83140 LUMO: -0.17960 factor:1 | 1 (-0.43492) | -1 | -1 |
| G: -6257.17264 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.24030 HOMO: -6.28855 LUMO: 0.01088 factor:1 | 1 (-0.70197) | -1 | -1 |
| G: -6257.17264 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.18701 HOMO: -6.31576 LUMO: 0.25307 factor:1 | 1 (-1.64868) | -1 | -1 |
| G: -6257.17264 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12524.05171 HOMO: -7.06408 LUMO: -2.76196 factor:1 | 1 (-2.51338) | -1 | -1 |
| G: -6257.17264 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.99575 HOMO: -5.95657 LUMO: 0.37552 factor:1 | 1 (-1.45741) | -1 | -1 |
| G: -6257.17264 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.07961 HOMO: -6.61781 LUMO: 0.02721 factor:1 | 1 (-1.54128) | -1 | -1 |
| G: -6257.17264 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.27502 HOMO: -6.26678 LUMO: -0.66668 factor:1 | 1 (-1.73669) | -1 | -1 |
| G: -6257.17264 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.82293 HOMO: -6.00011 LUMO: -0.13334 factor:1 | 1 (-1.28460) | -1 | -1 |
| G: -6257.17264 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.90540 HOMO: -5.60555 LUMO: 0.67484 factor:1 | 1 (-1.36707) | -1 | -1 |
| G: -6257.17264 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.65819 HOMO: -5.79875 LUMO: 0.99049 factor:1 | 1 (-1.11986) | -1 | -1 |
| G: -6257.17264 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.93803 HOMO: -5.97834 LUMO: 0.48436 factor:1 | 1 (-1.39970) | -1 | -1 |
| G: -6257.17264 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12520.94670 HOMO: -5.82868 LUMO: 0.91974 factor:1 | -1 (0.59163) | -1 | -1 |
| G: -6257.17264 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.98092 HOMO: -5.86677 LUMO: 0.99594 factor:1 | 1 (-0.44259) | -1 | -1 |
| G: -6257.17264 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.92179 HOMO: -5.70079 LUMO: 0.48980 factor:1 | 1 (-0.38346) | -1 | -1 |
| G: -6257.17264 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.12169 HOMO: -7.39605 LUMO: -1.02315 factor:1 | 1 (-0.58336) | 1 | -1 |
| G: -6257.17264 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.09069 HOMO: -7.22734 LUMO: -1.12927 factor:1 | 1 (-0.55236) | 1 | -1 |
| G: -6257.17264 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12520.69178 HOMO: -7.58926 LUMO: -0.65035 factor:1 | -1 (0.84655) | 1 | 1 |
| G: -6257.17264 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12520.09286 HOMO: -7.43959 LUMO: -0.75648 factor:1 | -1 (1.44547) | 1 | 1 |
| G: -6257.17264 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12520.62977 HOMO: -7.55388 LUMO: -1.15104 factor:1 | -1 (0.90856) | 1 | -1 |
| G: -6257.17264 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.24198 HOMO: -6.74570 LUMO: -2.85447 factor:1 | 1 (-1.70365) | -1 | -1 |
| G: -6257.17264 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.14054 HOMO: -7.35524 LUMO: -1.25444 factor:1 | 1 (-1.60221) | 1 | 1 |
| G: -6257.17264 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.34397 HOMO: -6.81645 LUMO: -1.20819 factor:1 | 1 (-1.80564) | -1 | -1 |
| G: -6257.17264 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.41889 HOMO: -6.99605 LUMO: -1.62996 factor:1 | 1 (-0.88056) | -1 | -1 |
| G: -6257.17264 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.94424 HOMO: -6.88992 LUMO: -0.47620 factor:1 | 1 (-0.40591) | -1 | -1 |
| G: -6257.17264 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.86000 HOMO: -7.22190 LUMO: -0.01905 factor:1 | 1 (-0.32167) | 1 | 1 |
| G: -6257.17264 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.07510 HOMO: -6.77836 LUMO: -0.82995 factor:1 | 1 (-0.53677) | -1 | -1 |
| G: -6257.17264 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.02215 HOMO: -6.48447 LUMO: -0.95512 factor:1 | 1 (-0.48382) | -1 | -1 |
| G: -6257.17264 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12520.88988 HOMO: -7.81239 LUMO: 1.22179 factor:1 | -1 (0.64845) | 1 | 1 |
| G: -6257.17264 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.05395 HOMO: -7.36612 LUMO: 0.19320 factor:1 | 1 (-1.51562) | 1 | 1 |
| G: -6257.17264 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.14029 HOMO: -7.24095 LUMO: 0.33470 factor:1 | 1 (-1.60196) | 1 | 1 |
| G: -6257.17264 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.19355 HOMO: -7.15932 LUMO: -2.24222 factor:1 | 1 (-0.65522) | -1 | -1 |
| G: -6257.17264 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.99779 HOMO: -6.88992 LUMO: -2.69937 factor:1 | 1 (-1.45946) | -1 | -1 |
| G: -6257.17264 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.11897 HOMO: -6.97428 LUMO: -0.98233 factor:1 | 1 (-0.58064) | -1 | -1 |
| G: -6257.17264 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.18685 HOMO: -7.17564 LUMO: -0.93879 factor:1 | 1 (-1.64852) | 1 | 1 |
| G: -6257.17264 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.31968 HOMO: -6.81645 LUMO: -1.14288 factor:1 | 1 (-0.78135) | -1 | -1 |
| G: -6257.17264 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.33777 HOMO: -6.83006 LUMO: -0.63403 factor:1 | 1 (-0.79944) | -1 | -1 |
| G: -6257.17264 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.41903 HOMO: -7.17292 LUMO: -1.07213 factor:1 | 1 (-0.88070) | 1 | 1 |
| G: -6257.17264 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.09549 HOMO: -7.53755 LUMO: 0.15510 factor:1 | -1 (0.44284) | 1 | 1 |
| G: -6257.17264 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.74199 HOMO: -6.50080 LUMO: -0.51702 factor:1 | 1 (-2.20366) | -1 | -1 |
| G: -6257.17264 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.86366 HOMO: -6.72665 LUMO: -0.80001 factor:1 | 1 (-1.32533) | -1 | -1 |
| G: -6257.17264 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.04625 HOMO: -6.72665 LUMO: 1.68711 factor:1 | 1 (-1.50792) | -1 | -1 |
| G: -6257.17264 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.90731 HOMO: -7.11850 LUMO: -0.75103 factor:1 | 1 (-1.36898) | 1 | 1 |
| G: -6257.17264 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.10924 HOMO: -6.87087 LUMO: -0.85988 factor:1 | 1 (-1.57091) | -1 | -1 |
| G: -6257.17264 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.01285 HOMO: -7.08857 LUMO: -0.89798 factor:1 | -1 (0.52548) | 1 | 1 |
| G: -6257.50192 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.83319 HOMO: -6.71305 LUMO: -0.85444 factor:1 | -1 (0.03442) | -1 | -1 |
| G: -6257.50192 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.90577 HOMO: -6.59332 LUMO: -0.60137 factor:1 | 1 (-0.03815) | -1 | -1 |
| G: -6257.50192 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12520.81143 HOMO: -7.28993 LUMO: 0.03265 factor:1 | -1 (1.05618) | 1 | 1 |
| G: -6257.50192 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12520.76632 HOMO: -7.32258 LUMO: 0.13878 factor:1 | -1 (1.10130) | 1 | 1 |
| G: -6257.50192 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12520.79222 HOMO: -7.28993 LUMO: 0.11429 factor:1 | -1 (1.07539) | 1 | 1 |
| G: -6257.50192 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.52764 HOMO: -6.86271 LUMO: -1.03947 factor:1 | -1 (0.33998) | -1 | -1 |
| G: -6257.50192 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.26042 HOMO: -6.55794 LUMO: -0.84900 factor:1 | -1 (0.60719) | -1 | -1 |
| G: -6257.50192 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.79540 HOMO: -7.03686 LUMO: 0.11429 factor:1 | -1 (0.07222) | -1 | -1 |
| G: -6257.50192 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.37977 HOMO: -7.06952 LUMO: -0.96056 factor:1 | -1 (0.48785) | 1 | 1 |
| G: -6257.50192 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.89148 HOMO: -6.90897 LUMO: -0.99866 factor:1 | 1 (-0.02386) | -1 | -1 |
| G: -6257.50192 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.89268 HOMO: -7.00693 LUMO: -0.83539 factor:1 | 1 (-0.02506) | -1 | -1 |
| G: -6257.50192 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.73235 HOMO: -6.74298 LUMO: -0.85172 factor:1 | -1 (0.13527) | -1 | -1 |
| G: -6257.50192 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.85232 HOMO: -6.83822 LUMO: -1.07213 factor:1 | -1 (0.01529) | -1 | -1 |
| G: -6257.50192 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.83923 HOMO: -7.21918 LUMO: -1.55377 factor:1 | -1 (0.02838) | 1 | 1 |
| G: -6257.50192 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.54867 HOMO: -6.84094 LUMO: -1.09934 factor:1 | -1 (0.31894) | -1 | -1 |
| G: -6257.50192 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.84936 HOMO: -7.09129 LUMO: -0.85988 factor:1 | -1 (0.01826) | 1 | 1 |
| G: -6257.50192 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.63082 HOMO: -6.57971 LUMO: -2.27215 factor:1 | -1 (0.23679) | -1 | -1 |
| G: -6257.50192 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.77570 HOMO: -6.81373 LUMO: -1.86942 factor:1 | -1 (0.09192) | -1 | -1 |
| G: -6257.50192 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.90125 HOMO: -6.59060 LUMO: -2.30480 factor:1 | 1 (-0.03363) | -1 | -1 |
| G: -6257.50192 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.91543 HOMO: -6.72938 LUMO: -1.23540 factor:1 | 1 (-0.04781) | -1 | -1 |
| G: -6257.50192 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.90963 HOMO: -6.94707 LUMO: -2.62318 factor:1 | 1 (-0.04201) | -1 | -1 |
| G: -6257.50192 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.70187 HOMO: -7.28177 LUMO: -0.09796 factor:1 | -1 (0.16574) | 1 | 1 |
| G: -6257.50192 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.78941 HOMO: -6.80013 LUMO: -0.79729 factor:1 | -1 (0.07821) | -1 | -1 |
| G: -6257.50192 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.56812 HOMO: -7.26544 LUMO: 0.12789 factor:1 | 1 (-0.70050) | 1 | 1 |
| G: -6257.50192 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.50893 HOMO: -6.51713 LUMO: -0.49253 factor:1 | 1 (-0.64132) | -1 | -1 |
| G: -6257.50192 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.55459 HOMO: -6.68856 LUMO: -0.77280 factor:1 | 1 (-0.68698) | -1 | -1 |
| G: -6257.50192 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.59323 HOMO: -6.41100 LUMO: -0.70750 factor:1 | 1 (-0.72562) | -1 | -1 |
| G: -6257.50192 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.44588 HOMO: -7.56204 LUMO: 0.22041 factor:1 | 1 (-0.57827) | 1 | 1 |
| G: -6257.50192 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.45884 HOMO: -6.68312 LUMO: 1.30343 factor:1 | 1 (-0.59122) | -1 | -1 |
| G: -6257.50192 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.18817 HOMO: -7.24367 LUMO: 0.17415 factor:1 | 1 (-0.32055) | 1 | 1 |
| G: -6257.50192 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.36762 HOMO: -7.52395 LUMO: 1.16737 factor:1 | 1 (-0.50001) | 1 | 1 |
| G: -6257.50192 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.61168 HOMO: -6.89264 LUMO: 0.23130 factor:1 | 1 (-0.74407) | -1 | -1 |
| G: -6257.50192 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.49402 HOMO: -7.21102 LUMO: 0.19048 factor:1 | 1 (-0.62641) | 1 | 1 |
| G: -6257.50192 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.35258 HOMO: -7.08312 LUMO: 0.25034 factor:1 | 1 (-0.48496) | 1 | 1 |
| G: -6257.50192 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.32752 HOMO: -6.49536 LUMO: -0.65852 factor:1 | 1 (-0.45990) | -1 | -1 |
| G: -6257.50192 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.39737 HOMO: -6.85455 LUMO: 0.13606 factor:1 | 1 (-0.52975) | -1 | -1 |
| G: -6257.50192 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.41280 HOMO: -7.10217 LUMO: 0.35919 factor:1 | 1 (-0.54518) | 1 | 1 |
| G: -6257.50192 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.12716 HOMO: -7.77429 LUMO: 1.19186 factor:1 | 1 (-0.25954) | 1 | 1 |
| G: -6257.50192 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.31497 HOMO: -6.57427 LUMO: -0.50069 factor:1 | 1 (-0.44736) | -1 | -1 |
| G: -6257.50192 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.90392 HOMO: -7.36340 LUMO: 0.10068 factor:1 | 1 (-0.03630) | 1 | 1 |
| G: -6257.50192 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.67308 HOMO: -7.28177 LUMO: 0.15238 factor:1 | -1 (0.19453) | 1 | 1 |
| G: -6257.50192 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.78808 HOMO: -6.86543 LUMO: -0.84355 factor:1 | -1 (0.07954) | -1 | -1 |
| G: -6257.50192 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.57552 HOMO: -6.55794 LUMO: 1.39594 factor:1 | 1 (-0.70790) | -1 | -1 |
| G: -6257.50192 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.68622 HOMO: -6.26134 LUMO: 1.53744 factor:1 | 1 (-0.81860) | -1 | -1 |
| G: -6257.50192 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.38402 HOMO: -5.97562 LUMO: 1.42316 factor:1 | 1 (-1.51641) | -1 | -1 |
| G: -6257.50192 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.30242 HOMO: -6.65046 LUMO: 1.44492 factor:1 | 1 (-1.43480) | -1 | -1 |
| G: -6257.50192 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.69574 HOMO: -6.92258 LUMO: 0.17415 factor:1 | 1 (-0.82812) | -1 | -1 |
| G: -6257.50192 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.32936 HOMO: -7.40966 LUMO: 0.19592 factor:1 | 1 (-1.46174) | 1 | 1 |
| G: -6257.50192 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.31957 HOMO: -7.17564 LUMO: 0.16871 factor:1 | 1 (-0.45195) | 1 | 1 |
| G: -6257.50192 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.81588 HOMO: -7.46953 LUMO: 0.22313 factor:1 | 1 (-0.94826) | 1 | 1 |
| G: -6257.50192 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.06478 HOMO: -6.13345 LUMO: 1.85854 factor:1 | 1 (-1.19716) | -1 | -1 |
| G: -6257.50192 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.50357 HOMO: -6.99333 LUMO: -1.65717 factor:1 | 1 (-0.63596) | -1 | -1 |
| G: -6257.50192 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.73511 HOMO: -6.93074 LUMO: -1.79323 factor:1 | 1 (-1.86749) | -1 | -1 |
| G: -6257.50192 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.69759 HOMO: -6.87904 LUMO: -1.79323 factor:1 | 1 (-0.82997) | -1 | -1 |
| G: -6257.50192 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.50123 HOMO: -6.84094 LUMO: 0.66940 factor:1 | 1 (-0.63362) | -1 | -1 |
| G: -6257.50192 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.63628 HOMO: -7.13210 LUMO: -1.17553 factor:1 | 1 (-0.76867) | 1 | 1 |
| G: -6257.50192 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.47897 HOMO: -6.52801 LUMO: -2.23678 factor:1 | 1 (-0.61136) | -1 | -1 |
| G: -6257.50192 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.35878 HOMO: -6.81917 LUMO: -1.86398 factor:1 | 1 (-0.49117) | -1 | -1 |
| G: -6257.50192 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.65881 HOMO: -7.30626 LUMO: -1.66806 factor:1 | 1 (-0.79120) | 1 | 1 |
| G: -6257.50192 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.91561 HOMO: -6.98516 LUMO: -1.40683 factor:1 | 1 (-1.04799) | -1 | -1 |
| G: -6257.50192 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.69462 HOMO: -6.95523 LUMO: -0.97145 factor:1 | 1 (-0.82701) | -1 | -1 |
| G: -6257.50192 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.78622 HOMO: -6.83278 LUMO: -2.68848 factor:1 | 1 (-0.91860) | -1 | -1 |
| G: -6257.50192 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.99569 HOMO: -7.25456 LUMO: -2.97420 factor:1 | 1 (-1.12808) | -1 | -1 |
| G: -6257.50192 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.66808 HOMO: -6.80557 LUMO: -2.65039 factor:1 | 1 (-1.80047) | -1 | -1 |
| G: -6257.50192 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.46773 HOMO: -7.10489 LUMO: 0.77008 factor:1 | 1 (-1.60011) | 1 | -1 |
| G: -6257.50192 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.50604 HOMO: -7.28993 LUMO: -1.06124 factor:1 | 1 (-1.63842) | 1 | 1 |
| G: -6257.50192 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.81286 HOMO: -7.11578 LUMO: -1.10206 factor:1 | 1 (-0.94524) | 1 | 1 |
| G: -6257.50192 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.92938 HOMO: -6.91713 LUMO: -1.36329 factor:1 | 1 (-1.06176) | -1 | -1 |
| G: -6257.50192 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.93414 HOMO: -7.07224 LUMO: 0.51974 factor:1 | 1 (-1.06652) | 1 | 1 |
| G: -6257.50192 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.53280 HOMO: -7.22734 LUMO: -0.93335 factor:1 | 1 (-0.66518) | 1 | 1 |
| G: -6257.50192 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.39371 HOMO: -7.19469 LUMO: -0.96600 factor:1 | 1 (-1.52610) | 1 | 1 |
| G: -6257.50192 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.27393 HOMO: -6.93890 LUMO: -0.66940 factor:1 | 1 (-1.40631) | -1 | -1 |
| G: -6257.50192 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.81885 HOMO: -7.09673 LUMO: -1.05852 factor:1 | -1 (0.04876) | 1 | 1 |
| G: -6257.50192 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.80868 HOMO: -7.19197 LUMO: -2.26943 factor:1 | -1 (0.05894) | -1 | -1 |
| G: -6257.50192 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.74021 HOMO: -6.90081 LUMO: -2.64767 factor:1 | -1 (0.12740) | -1 | -1 |
| G: -6257.50192 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.69852 HOMO: -6.93890 LUMO: -2.65039 factor:1 | 1 (-0.83090) | -1 | -1 |
| G: -6257.50192 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.50809 HOMO: -6.80013 LUMO: -2.54154 factor:1 | 1 (-0.64047) | -1 | -1 |
| G: -6257.50192 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.79768 HOMO: -6.68040 LUMO: -0.89798 factor:1 | -1 (0.06993) | -1 | -1 |
| G: -6257.50192 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.81499 HOMO: -7.01782 LUMO: -1.09662 factor:1 | -1 (0.05263) | -1 | -1 |
| G: -6257.50192 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.59473 HOMO: -6.58516 LUMO: -0.83539 factor:1 | 1 (-0.72712) | -1 | -1 |
| G: -6257.50192 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.45378 HOMO: -7.46953 LUMO: 0.06259 factor:1 | 1 (-0.58616) | 1 | 1 |
| G: -6257.50192 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.58011 HOMO: -6.96884 LUMO: -0.99866 factor:1 | 1 (-1.71249) | -1 | -1 |
| G: -6257.50192 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.79966 HOMO: -7.29809 LUMO: -0.19320 factor:1 | 1 (-0.93204) | 1 | 1 |
| G: -6257.50192 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.81185 HOMO: -6.86271 LUMO: 0.04082 factor:1 | 1 (-0.94424) | -1 | -1 |
| G: -6257.50192 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.70999 HOMO: -6.36746 LUMO: -1.02587 factor:1 | 1 (-1.84237) | -1 | -1 |
| G: -6257.50192 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.97770 HOMO: -7.15659 LUMO: -1.25989 factor:1 | 1 (-2.11008) | 1 | 1 |
| G: -6257.50192 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.59060 HOMO: -6.69128 LUMO: -0.59865 factor:1 | 1 (-0.72298) | -1 | -1 |
| G: -6257.50192 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.97187 HOMO: -7.09129 LUMO: -1.08573 factor:1 | 1 (-2.10426) | 1 | 1 |
| G: -6257.50192 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.61695 HOMO: -6.64502 LUMO: -0.66396 factor:1 | 1 (-1.74934) | -1 | -1 |
| G: -6257.50192 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.84665 HOMO: -6.93346 LUMO: -0.87349 factor:1 | 1 (-0.97904) | -1 | -1 |
| G: -6257.50192 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.24233 HOMO: -6.77019 LUMO: -0.87349 factor:1 | 1 (-1.37472) | -1 | -1 |
| G: -6257.50192 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.28084 HOMO: -6.59060 LUMO: -0.82995 factor:1 | 1 (-1.41322) | -1 | -1 |
| G: -6257.50192 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.20555 HOMO: -7.17564 LUMO: -1.08846 factor:1 | 1 (-1.33793) | 1 | 1 |
| G: -6257.50192 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.65236 HOMO: -7.27088 LUMO: -1.18642 factor:1 | 1 (-0.78475) | 1 | 1 |
| G: -6257.50192 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.22304 HOMO: -7.06680 LUMO: -1.13199 factor:1 | 1 (-1.35543) | 1 | 1 |
| G: -6257.50192 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.98698 HOMO: -7.21918 LUMO: -1.03947 factor:1 | 1 (-1.11937) | 1 | 1 |
| G: -6257.50192 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.11711 HOMO: -7.26000 LUMO: -0.11973 factor:1 | 1 (-1.24949) | 1 | 1 |
| G: -6257.50192 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.16505 HOMO: -6.77564 LUMO: 0.23402 factor:1 | 1 (-1.29744) | -1 | -1 |
| G: -6257.50192 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.71489 HOMO: -7.07224 LUMO: -0.75648 factor:1 | 1 (-1.84727) | 1 | 1 |
| G: -6257.50192 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12524.16415 HOMO: -7.45048 LUMO: 0.18232 factor:1 | 1 (-2.29653) | 1 | 1 |
| G: -6257.50192 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.62066 HOMO: -7.48313 LUMO: 0.15238 factor:1 | 1 (-0.75305) | 1 | 1 |
| G: -6257.50192 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.17994 HOMO: -6.60692 LUMO: -0.50885 factor:1 | 1 (-1.31232) | -1 | -1 |
| G: -6257.50192 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.24489 HOMO: -6.62869 LUMO: -0.60954 factor:1 | 1 (-1.37728) | -1 | -1 |
| G: -6257.50192 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.13295 HOMO: -7.40422 LUMO: -1.28982 factor:1 | 1 (-1.26533) | 1 | 1 |
| G: -6257.50192 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.24233 HOMO: -6.75114 LUMO: -1.23268 factor:1 | 1 (-1.37472) | -1 | -1 |
| G: -6257.50192 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12524.11865 HOMO: -6.84638 LUMO: -0.73199 factor:1 | 1 (-2.25103) | -1 | -1 |
| G: -6257.50192 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.84558 HOMO: -6.79196 LUMO: -1.43676 factor:1 | 1 (-1.97797) | -1 | -1 |
| G: -6257.50192 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.25357 HOMO: -7.00965 LUMO: -1.37690 factor:1 | 1 (-1.38596) | -1 | -1 |
| G: -6257.50192 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.25643 HOMO: -6.97972 LUMO: -1.58098 factor:1 | 1 (-1.38881) | -1 | -1 |
| G: -6257.50192 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.05486 HOMO: -6.91169 LUMO: -1.48574 factor:1 | 1 (-0.18724) | -1 | -1 |
| G: -6257.50192 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.13817 HOMO: -6.90081 LUMO: -1.30343 factor:1 | 1 (-1.27055) | -1 | -1 |
| G: -6257.50192 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.03760 HOMO: -6.78652 LUMO: -1.51840 factor:1 | 1 (-1.16998) | -1 | -1 |
| G: -6257.50192 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12524.48108 HOMO: -6.84638 LUMO: -1.15104 factor:1 | 1 (-2.61346) | -1 | -1 |
| G: -6257.50192 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.42903 HOMO: -6.61237 LUMO: -0.89798 factor:1 | 1 (-1.56142) | -1 | -1 |
| G: -6257.50192 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.99322 HOMO: -7.16204 LUMO: -1.30070 factor:1 | 1 (-0.12561) | 1 | 1 |
| G: -6257.50192 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.10179 HOMO: -7.32803 LUMO: 0.14694 factor:1 | 1 (-1.23417) | 1 | 1 |
| G: -6257.50192 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.97976 HOMO: -6.99877 LUMO: -0.87621 factor:1 | 1 (-2.11215) | -1 | -1 |
| G: -6257.50192 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.20321 HOMO: -6.99877 LUMO: -0.97145 factor:1 | 1 (-1.33559) | -1 | -1 |
| G: -6257.50192 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.07561 HOMO: -7.08040 LUMO: -1.09662 factor:1 | 1 (-1.20800) | 1 | 1 |
| G: -6257.50192 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12524.09479 HOMO: -6.90897 LUMO: -1.14016 factor:1 | 1 (-2.22717) | -1 | -1 |
| G: -6257.50192 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.56091 HOMO: -6.68312 LUMO: -0.74831 factor:1 | 1 (-0.69329) | -1 | -1 |
| G: -6257.50192 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.65808 HOMO: -6.99061 LUMO: -0.86804 factor:1 | 1 (-0.79046) | -1 | -1 |
| G: -6257.50192 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.38912 HOMO: -7.10761 LUMO: -1.18642 factor:1 | 1 (-0.52151) | 1 | 1 |
| G: -6257.50192 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.48639 HOMO: -6.79196 LUMO: -0.71294 factor:1 | 1 (-1.61878) | -1 | -1 |
| G: -6257.50192 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.12356 HOMO: -6.86271 LUMO: -0.81362 factor:1 | 1 (-1.25594) | -1 | -1 |
| G: -6257.50192 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.41271 HOMO: -7.01510 LUMO: -0.99322 factor:1 | 1 (-0.54510) | -1 | -1 |
| G: -6257.50192 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.59293 HOMO: -6.88720 LUMO: -0.87893 factor:1 | 1 (-1.72531) | -1 | -1 |
| G: -6257.50192 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.08286 HOMO: -6.88448 LUMO: 0.22041 factor:1 | 1 (-0.21524) | -1 | -1 |
| G: -6257.50192 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.51328 HOMO: -7.55932 LUMO: 1.12111 factor:1 | 1 (-1.64566) | 1 | 1 |
| G: -6257.50192 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.60080 HOMO: -6.46815 LUMO: -0.86260 factor:1 | 1 (-0.73318) | -1 | -1 |
| G: -6257.50192 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.87530 HOMO: -7.13755 LUMO: 0.23130 factor:1 | 1 (-2.00768) | 1 | 1 |
| G: -6257.50192 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.39687 HOMO: -6.78924 LUMO: 1.51023 factor:1 | 1 (-1.52925) | -1 | -1 |
| G: -6257.50192 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.22257 HOMO: -6.48992 LUMO: 1.74969 factor:1 | -1 (0.64505) | -1 | -1 |
| G: -6257.50192 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.22681 HOMO: -6.78380 LUMO: 1.81500 factor:1 | 1 (-0.35919) | -1 | -1 |
| G: -6257.50192 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.36899 HOMO: -6.49536 LUMO: 1.70615 factor:1 | 1 (-0.50137) | -1 | -1 |
| G: -6257.50192 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.14923 HOMO: -6.38651 LUMO: 1.44492 factor:1 | 1 (-0.28161) | -1 | -1 |
| G: -6257.50192 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.08909 HOMO: -6.83822 LUMO: 1.38234 factor:1 | 1 (-0.22147) | -1 | -1 |
| G: -6257.50192 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.23448 HOMO: -6.01644 LUMO: 1.20274 factor:1 | 1 (-0.36686) | -1 | -1 |
| G: -6257.50192 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.62151 HOMO: -6.18243 LUMO: 1.77962 factor:1 | 1 (-0.75389) | -1 | -1 |
| G: -6257.50192 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.26126 HOMO: -6.81917 LUMO: -1.01771 factor:1 | 1 (-0.39364) | -1 | -1 |
| G: -6257.50192 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.64109 HOMO: -6.61237 LUMO: -0.91702 factor:1 | 1 (-1.77347) | -1 | -1 |
| G: -6257.50192 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.09920 HOMO: -6.84094 LUMO: -0.84900 factor:1 | 1 (-1.23159) | -1 | -1 |
| G: -6257.50192 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.65916 HOMO: -6.81917 LUMO: -1.01771 factor:1 | 1 (-1.79154) | -1 | -1 |
| G: -6257.50192 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.94339 HOMO: -7.86953 LUMO: 1.16737 factor:1 | 1 (-1.07577) | 1 | 1 |
| G: -6257.50192 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.15041 HOMO: -7.40694 LUMO: 0.11429 factor:1 | 1 (-1.28280) | 1 | 1 |
| G: -6257.50192 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.33624 HOMO: -6.70489 LUMO: -0.65035 factor:1 | 1 (-1.46863) | -1 | -1 |
| G: -6257.50192 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.47502 HOMO: -7.23279 LUMO: 0.33470 factor:1 | 1 (-1.60740) | 1 | 1 |
| G: -6257.50192 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.56104 HOMO: -7.17020 LUMO: 0.41361 factor:1 | 1 (-0.69343) | 1 | 1 |
| G: -6257.50192 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.72020 HOMO: -6.90353 LUMO: -0.90070 factor:1 | 1 (-0.85259) | -1 | -1 |
| G: -6257.50192 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.78156 HOMO: -7.39061 LUMO: 0.17687 factor:1 | 1 (-0.91395) | 1 | 1 |
| G: -6257.50192 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.57699 HOMO: -7.16748 LUMO: 0.42178 factor:1 | 1 (-0.70937) | 1 | 1 |
| G: -6257.50192 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.38839 HOMO: -7.36884 LUMO: -1.11295 factor:1 | 1 (-0.52077) | 1 | 1 |
| G: -6257.50192 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.39329 HOMO: -7.33347 LUMO: 0.33198 factor:1 | 1 (-0.52567) | 1 | 1 |
| G: -6257.50192 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.82047 HOMO: -7.31986 LUMO: -0.83539 factor:1 | 1 (-1.95285) | 1 | 1 |
| G: -6257.50192 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.47685 HOMO: -7.31170 LUMO: 0.08708 factor:1 | 1 (-0.60924) | 1 | 1 |
| G: -6257.50192 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.13841 HOMO: -7.36884 LUMO: 0.38096 factor:1 | 1 (-1.27080) | 1 | 1 |
| G: -6257.50192 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.79826 HOMO: -6.99333 LUMO: 1.74153 factor:1 | 1 (-1.93065) | -1 | -1 |
| G: -6257.50192 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.98444 HOMO: -6.94435 LUMO: 1.74969 factor:1 | 1 (-2.11683) | -1 | -1 |
| G: -6257.50192 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.50607 HOMO: -7.02598 LUMO: 1.43404 factor:1 | 1 (-1.63845) | -1 | -1 |
| G: -6257.50192 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.02494 HOMO: -6.41100 LUMO: 1.62996 factor:1 | 1 (-1.15733) | -1 | -1 |
| G: -6257.50192 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.10429 HOMO: -6.57699 LUMO: 1.81228 factor:1 | 1 (-1.23668) | -1 | -1 |
| G: -6257.50192 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.16081 HOMO: -6.86543 LUMO: 1.49935 factor:1 | 1 (-1.29319) | -1 | -1 |
| G: -6257.50192 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.27447 HOMO: -6.91169 LUMO: -1.22451 factor:1 | 1 (-1.40686) | -1 | -1 |
| G: -6257.50192 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.30965 HOMO: -7.09945 LUMO: -1.23812 factor:1 | -1 (0.55797) | 1 | 1 |
| G: -6257.50192 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.41328 HOMO: -7.48857 LUMO: 0.10340 factor:1 | 1 (-1.54566) | 1 | 1 |
| G: -6257.50192 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.02000 HOMO: -7.21918 LUMO: -0.06803 factor:1 | 1 (-0.15238) | 1 | 1 |
| G: -6257.50192 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.52716 HOMO: -6.34025 LUMO: -0.68845 factor:1 | 1 (-1.65954) | -1 | -1 |
| G: -6257.50192 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.02902 HOMO: -6.82734 LUMO: -0.77825 factor:1 | 1 (-1.16141) | -1 | -1 |
| G: -6257.50192 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12520.54305 HOMO: -6.92258 LUMO: -1.03675 factor:1 | -1 (1.32457) | -1 | -1 |
| G: -6257.50192 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12520.91228 HOMO: -6.42461 LUMO: -0.95240 factor:1 | -1 (0.95534) | -1 | -1 |
| G: -6257.50192 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.68272 HOMO: -6.96067 LUMO: -1.05036 factor:1 | 1 (-1.81511) | -1 | -1 |
| G: -6257.50192 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.79354 HOMO: -7.23551 LUMO: 0.12245 factor:1 | 1 (-0.92592) | 1 | 1 |
| G: -6257.50192 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.31045 HOMO: -6.85183 LUMO: 0.16055 factor:1 | 1 (-0.44284) | -1 | -1 |
| G: -6257.50192 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.36956 HOMO: -6.46815 LUMO: -0.89253 factor:1 | 1 (-0.50194) | -1 | -1 |
| G: -6257.50192 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.38625 HOMO: -7.23823 LUMO: -0.06259 factor:1 | -1 (0.48137) | 1 | 1 |
| G: -6257.50192 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.29485 HOMO: -6.76475 LUMO: -0.99049 factor:1 | 1 (-1.42724) | -1 | -1 |
| G: -6257.50192 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.43872 HOMO: -7.14843 LUMO: -0.88165 factor:1 | 1 (-1.57110) | 1 | 1 |
| G: -6257.50192 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.56243 HOMO: -7.15659 LUMO: 0.20681 factor:1 | 1 (-0.69482) | 1 | 1 |
| G: -6257.50192 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.74015 HOMO: -7.11306 LUMO: 0.14150 factor:1 | 1 (-0.87253) | 1 | 1 |
| G: -6257.50192 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.62464 HOMO: -6.67223 LUMO: -0.86260 factor:1 | 1 (-0.75702) | -1 | -1 |
| G: -6257.50192 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.26097 HOMO: -6.92530 LUMO: 0.30749 factor:1 | -1 (0.60665) | -1 | -1 |
| G: -6257.50192 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.48463 HOMO: -6.50624 LUMO: -0.70477 factor:1 | 1 (-0.61702) | -1 | -1 |
| G: -6257.50192 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.48039 HOMO: -7.35524 LUMO: 0.75103 factor:1 | 1 (-0.61277) | 1 | 1 |
| G: -6257.50192 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.75873 HOMO: -7.07768 LUMO: -0.26939 factor:1 | 1 (-0.89112) | 1 | 1 |
| G: -6257.50192 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.23889 HOMO: -7.15932 LUMO: 0.42450 factor:1 | 1 (-0.37127) | 1 | 1 |
| G: -6257.50192 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.34235 HOMO: -7.46136 LUMO: 0.04626 factor:1 | 1 (-0.47473) | 1 | 1 |
| G: -6257.50192 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.04569 HOMO: -7.05047 LUMO: -1.06669 factor:1 | 1 (-0.17807) | -1 | -1 |
| G: -6257.50192 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12520.73374 HOMO: -6.66951 LUMO: -0.99322 factor:1 | -1 (1.13387) | -1 | -1 |
| G: -6257.50192 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.25737 HOMO: -7.01782 LUMO: -1.08846 factor:1 | -1 (0.61024) | -1 | -1 |
| G: -6257.50192 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.45082 HOMO: -7.03959 LUMO: -1.15376 factor:1 | -1 (0.41680) | -1 | -1 |
| G: -6257.50192 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.54029 HOMO: -6.68856 LUMO: 1.61364 factor:1 | -1 (0.32733) | -1 | -1 |
| G: -6257.50192 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.82952 HOMO: -6.53345 LUMO: 1.60275 factor:1 | -1 (0.03810) | -1 | -1 |
| G: -6257.50192 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.08544 HOMO: -6.73482 LUMO: 1.86398 factor:1 | 1 (-0.21783) | -1 | -1 |
| G: -6257.50192 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.04616 HOMO: -6.87632 LUMO: 1.59731 factor:1 | -1 (0.82146) | -1 | -1 |
| G: -6257.50192 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.20540 HOMO: -6.31848 LUMO: 2.12521 factor:1 | -1 (0.66222) | -1 | -1 |
| G: -6257.50192 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.24671 HOMO: -6.35114 LUMO: 1.71432 factor:1 | -1 (0.62091) | -1 | -1 |
| G: -6257.50192 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.23742 HOMO: -6.34842 LUMO: 1.92929 factor:1 | 1 (-0.36980) | -1 | -1 |
| G: -6257.50192 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.56269 HOMO: -6.14977 LUMO: 1.78235 factor:1 | 1 (-1.69508) | -1 | -1 |
| G: -6257.50192 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.60192 HOMO: -6.31032 LUMO: 1.51567 factor:1 | 1 (-0.73430) | -1 | -1 |
| G: -6257.50192 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12520.36313 HOMO: -6.25862 LUMO: 1.75241 factor:1 | -1 (1.50449) | -1 | -1 |
| G: -6257.50192 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.43479 HOMO: -6.49264 LUMO: 1.66806 factor:1 | -1 (0.43282) | -1 | -1 |
| G: -6257.50192 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.00142 HOMO: -6.28311 LUMO: 1.60003 factor:1 | -1 (0.86619) | -1 | -1 |
| G: -6257.50192 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.66427 HOMO: -7.13210 LUMO: -0.04354 factor:1 | -1 (0.20335) | 1 | 1 |
| G: -6257.50192 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.40231 HOMO: -7.35252 LUMO: 0.03537 factor:1 | 1 (-1.53469) | 1 | 1 |
| G: -6257.50192 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.47922 HOMO: -6.58243 LUMO: -0.48980 factor:1 | 1 (-0.61160) | -1 | -1 |
| G: -6257.50192 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.50408 HOMO: -6.90081 LUMO: -0.05442 factor:1 | 1 (-1.63647) | -1 | -1 |
| G: -6257.50192 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.71642 HOMO: -7.22734 LUMO: 0.17143 factor:1 | 1 (-0.84880) | 1 | 1 |
| G: -6257.50192 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.66023 HOMO: -7.13210 LUMO: -0.99866 factor:1 | 1 (-0.79261) | 1 | 1 |
| G: -6257.50192 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.37511 HOMO: -7.39878 LUMO: 0.13334 factor:1 | 1 (-0.50749) | 1 | 1 |
| G: -6257.50192 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.47870 HOMO: -7.04503 LUMO: -0.89798 factor:1 | 1 (-0.61109) | -1 | -1 |
| G: -6257.50192 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.43870 HOMO: -6.95523 LUMO: -1.07213 factor:1 | 1 (-0.57109) | -1 | -1 |
| G: -6257.50192 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.25854 HOMO: -6.75114 LUMO: -1.28438 factor:1 | -1 (0.60907) | -1 | -1 |
| G: -6257.50192 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.50145 HOMO: -6.75114 LUMO: -0.11701 factor:1 | 1 (-0.63383) | -1 | -1 |
| G: -6257.50192 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.18235 HOMO: -6.83278 LUMO: -0.01633 factor:1 | -1 (0.68526) | -1 | -1 |
| G: -6257.50192 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.70423 HOMO: -6.93890 LUMO: -0.88981 factor:1 | 1 (-0.83661) | -1 | -1 |
| G: -6257.50192 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.20158 HOMO: -7.07224 LUMO: -1.08573 factor:1 | 1 (-0.33397) | 1 | 1 |
| G: -6257.50192 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.03454 HOMO: -6.99877 LUMO: -0.95240 factor:1 | -1 (0.83308) | -1 | -1 |
| G: -6257.50192 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.13179 HOMO: -7.09129 LUMO: 0.35375 factor:1 | -1 (0.73582) | 1 | 1 |
| G: -6257.50192 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.84185 HOMO: -7.09401 LUMO: 0.04354 factor:1 | -1 (0.02577) | 1 | 1 |
| G: -6257.50192 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.21133 HOMO: -6.85183 LUMO: -0.68573 factor:1 | -1 (0.65628) | -1 | -1 |
| G: -6257.50192 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12524.31531 HOMO: -6.83006 LUMO: -0.58777 factor:1 | 1 (-2.44769) | -1 | -1 |
| G: -6257.50192 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12524.00643 HOMO: -7.40422 LUMO: 0.17687 factor:1 | 1 (-2.13881) | 1 | 1 |
| G: -6257.50192 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.29757 HOMO: -7.15932 LUMO: 0.10340 factor:1 | 1 (-1.42996) | 1 | 1 |
| G: -6257.50192 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12524.14532 HOMO: -7.03414 LUMO: -0.19592 factor:1 | 1 (-2.27770) | -1 | -1 |
| G: -6257.50192 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.90825 HOMO: -6.48447 LUMO: -0.36191 factor:1 | 1 (-2.04064) | -1 | -1 |
| G: -6257.50192 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.30064 HOMO: -7.49402 LUMO: 0.11429 factor:1 | -1 (0.56698) | 1 | 1 |
| G: -6257.50192 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.08240 HOMO: -7.01237 LUMO: -1.06397 factor:1 | 1 (-0.21478) | -1 | -1 |
| G: -6257.50192 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.17622 HOMO: -6.67223 LUMO: -1.07213 factor:1 | 1 (-0.30860) | -1 | -1 |
| G: -6257.50192 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.03513 HOMO: -7.38789 LUMO: -1.15376 factor:1 | 1 (-0.16751) | 1 | 1 |
| G: -6257.50192 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.85231 HOMO: -6.42461 LUMO: -1.23812 factor:1 | 1 (-1.98469) | -1 | -1 |
| G: -6257.50192 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12524.02009 HOMO: -7.36884 LUMO: -1.19186 factor:1 | 1 (-2.15248) | 1 | 1 |
| G: -6257.50192 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.12236 HOMO: -6.65591 LUMO: 0.07075 factor:1 | 1 (-1.25474) | -1 | -1 |
| G: -6257.50192 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.20231 HOMO: -7.39061 LUMO: -0.16871 factor:1 | 1 (-1.33469) | 1 | 1 |
| G: -6257.50192 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12524.28105 HOMO: -6.90353 LUMO: -0.96056 factor:1 | 1 (-2.41343) | -1 | -1 |
| G: -6257.50192 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.67486 HOMO: -7.42054 LUMO: 0.19048 factor:1 | 1 (-1.80724) | 1 | 1 |
| G: -6257.50192 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.08282 HOMO: -7.40150 LUMO: 0.35647 factor:1 | 1 (-1.21521) | 1 | 1 |
| G: -6257.50192 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.38213 HOMO: -6.56067 LUMO: -0.96056 factor:1 | 1 (-0.51451) | -1 | -1 |
| G: -6257.50192 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12524.17253 HOMO: -6.89809 LUMO: -0.81090 factor:1 | 1 (-2.30491) | -1 | -1 |
| G: -6257.50192 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.40182 HOMO: -6.91986 LUMO: -0.84900 factor:1 | 1 (-1.53421) | -1 | -1 |
| G: -6257.50192 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.92546 HOMO: -6.61509 LUMO: -0.62042 factor:1 | 1 (-1.05784) | -1 | -1 |
| G: -6257.50192 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.15452 HOMO: -6.58243 LUMO: -0.65579 factor:1 | 1 (-1.28691) | -1 | -1 |
| G: -6257.50192 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.32553 HOMO: -6.52257 LUMO: -0.92519 factor:1 | 1 (-0.45791) | -1 | -1 |
| G: -6257.50192 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.53766 HOMO: -6.69128 LUMO: 1.49118 factor:1 | 1 (-1.67004) | -1 | -1 |
| G: -6257.50192 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.18438 HOMO: -7.02870 LUMO: 1.67894 factor:1 | 1 (-0.31677) | -1 | -1 |
| G: -6257.50192 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.16040 HOMO: -6.88720 LUMO: 1.68711 factor:1 | 1 (-1.29279) | -1 | -1 |
| G: -6257.50192 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.40005 HOMO: -5.89943 LUMO: 1.03675 factor:1 | 1 (-1.53244) | -1 | -1 |
| G: -6257.50192 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.55070 HOMO: -6.40556 LUMO: 1.14560 factor:1 | 1 (-0.68309) | -1 | -1 |
| G: -6257.50192 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.77829 HOMO: -6.51168 LUMO: 1.48030 factor:1 | 1 (-1.91067) | -1 | -1 |
| G: -6257.50192 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.93286 HOMO: -6.64502 LUMO: 1.91568 factor:1 | 1 (-1.06524) | -1 | -1 |
| G: -6257.50192 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.30070 HOMO: -6.47903 LUMO: 1.91296 factor:1 | 1 (-1.43309) | -1 | -1 |
| G: -6257.50192 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.31005 HOMO: -6.34297 LUMO: 1.91840 factor:1 | -1 (0.55756) | -1 | -1 |
| G: -6257.50192 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.26711 HOMO: -6.89809 LUMO: 1.82861 factor:1 | -1 (0.60050) | -1 | -1 |
| G: -6257.50192 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.29242 HOMO: -6.10079 LUMO: 1.62996 factor:1 | -1 (0.57519) | -1 | -1 |
| G: -6257.50192 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.20790 HOMO: -7.16476 LUMO: -0.92247 factor:1 | -1 (0.65971) | 1 | 1 |
| G: -6257.50192 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.24287 HOMO: -7.10489 LUMO: -0.95784 factor:1 | -1 (0.62475) | 1 | 1 |
| G: -6257.50192 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.06706 HOMO: -6.76475 LUMO: -0.99866 factor:1 | -1 (0.80056) | -1 | -1 |
| G: -6257.50192 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.65471 HOMO: -6.81373 LUMO: -1.05036 factor:1 | 1 (-0.78709) | -1 | -1 |
| G: -6257.50192 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.70173 HOMO: -6.90081 LUMO: -1.03947 factor:1 | 1 (-0.83411) | -1 | -1 |
| G: -6257.50192 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.56679 HOMO: -7.06952 LUMO: -0.91702 factor:1 | 1 (-0.69917) | 1 | 1 |
| G: -6257.50192 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.42578 HOMO: -6.73482 LUMO: -0.94151 factor:1 | 1 (-0.55816) | -1 | -1 |
| G: -6257.50192 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.15988 HOMO: -6.99605 LUMO: -1.04764 factor:1 | 1 (-1.29227) | -1 | -1 |
| G: -6257.50192 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.09997 HOMO: -7.03686 LUMO: -0.93335 factor:1 | 1 (-1.23235) | -1 | -1 |
| G: -6257.50192 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.48609 HOMO: -6.81101 LUMO: -0.95240 factor:1 | 1 (-1.61848) | -1 | -1 |
| G: -6257.50192 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.53956 HOMO: -6.83822 LUMO: -0.65307 factor:1 | 1 (-1.67195) | -1 | -1 |
| G: -6257.50192 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.06223 HOMO: -7.05319 LUMO: -0.81634 factor:1 | 1 (-0.19462) | -1 | -1 |
| G: -6257.50192 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.13649 HOMO: -7.57565 LUMO: 0.19048 factor:1 | 1 (-0.26888) | 1 | 1 |
| G: -6257.50192 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.33712 HOMO: -6.56067 LUMO: -0.50613 factor:1 | 1 (-0.46951) | -1 | -1 |
| G: -6257.50192 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.24923 HOMO: -6.74298 LUMO: -0.70477 factor:1 | 1 (-0.38161) | -1 | -1 |
| G: -6257.50192 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.28477 HOMO: -7.02054 LUMO: 0.03537 factor:1 | 1 (-0.41715) | -1 | -1 |
| G: -6257.50192 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.41388 HOMO: -7.33347 LUMO: -0.17960 factor:1 | 1 (-0.54627) | 1 | 1 |
| G: -6257.50192 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.46442 HOMO: -6.98244 LUMO: -0.88165 factor:1 | 1 (-0.59680) | -1 | -1 |
| G: -6257.50192 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.13486 HOMO: -7.14843 LUMO: -1.19730 factor:1 | 1 (-0.26724) | 1 | 1 |
| G: -6257.50192 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.40681 HOMO: -7.17564 LUMO: -1.21907 factor:1 | 1 (-0.53919) | 1 | 1 |
| G: -6257.50192 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.14359 HOMO: -6.74026 LUMO: -0.86532 factor:1 | 1 (-0.27598) | -1 | -1 |
| G: -6257.50192 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.46768 HOMO: -6.82462 LUMO: -1.24084 factor:1 | 1 (-0.60007) | -1 | -1 |
| G: -6257.50192 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.03954 HOMO: -6.78924 LUMO: -0.70477 factor:1 | 1 (-0.17192) | -1 | -1 |
| G: -6257.50192 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.25200 HOMO: -7.41238 LUMO: 0.05987 factor:1 | 1 (-0.38439) | 1 | 1 |
| G: -6257.50192 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.46178 HOMO: -6.75931 LUMO: 0.02721 factor:1 | 1 (-0.59416) | -1 | -1 |
| G: -6257.50192 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.23777 HOMO: -6.28583 LUMO: -0.93063 factor:1 | 1 (-0.37016) | -1 | -1 |
| G: -6257.50192 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.49525 HOMO: -6.69128 LUMO: -0.83539 factor:1 | 1 (-0.62763) | -1 | -1 |
| G: -6257.50192 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.34406 HOMO: -7.22190 LUMO: 0.01361 factor:1 | 1 (-0.47644) | 1 | 1 |
| G: -6257.50192 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.18727 HOMO: -6.95251 LUMO: -1.09934 factor:1 | 1 (-0.31965) | -1 | -1 |
| G: -6257.50192 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.28207 HOMO: -6.75387 LUMO: -0.90614 factor:1 | 1 (-0.41446) | -1 | -1 |
| G: -6257.50192 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.24686 HOMO: -7.48585 LUMO: 0.05987 factor:1 | 1 (-0.37925) | 1 | 1 |
| G: -6257.50192 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.47070 HOMO: -6.92802 LUMO: -0.66940 factor:1 | 1 (-0.60309) | -1 | -1 |
| G: -6257.50192 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.79128 HOMO: -7.29537 LUMO: -0.14150 factor:1 | 1 (-0.92366) | 1 | 1 |
| G: -6257.50192 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.90350 HOMO: -6.57155 LUMO: -0.86804 factor:1 | 1 (-1.03588) | -1 | -1 |
| G: -6257.50192 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.99939 HOMO: -6.87632 LUMO: -0.77825 factor:1 | 1 (-1.13178) | -1 | -1 |
| G: -6257.50192 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.81604 HOMO: -6.45998 LUMO: -0.31565 factor:1 | 1 (-0.94843) | -1 | -1 |
| G: -6257.50192 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.87456 HOMO: -7.51306 LUMO: 0.05714 factor:1 | 1 (-2.00695) | 1 | 1 |
| G: -6257.50192 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12524.40500 HOMO: -6.86271 LUMO: -0.00816 factor:1 | 1 (-2.53738) | -1 | -1 |
| G: -6257.50192 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.54521 HOMO: -6.43277 LUMO: -1.07485 factor:1 | 1 (-0.67759) | -1 | -1 |
| G: -6257.50192 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.14380 HOMO: -6.78108 LUMO: -0.81362 factor:1 | 1 (-1.27619) | -1 | -1 |
| G: -6257.50192 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.17959 HOMO: -6.88448 LUMO: 1.21907 factor:1 | 1 (-1.31197) | -1 | -1 |
| G: -6257.50192 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.93278 HOMO: -6.97700 LUMO: 1.44765 factor:1 | 1 (-1.06516) | -1 | -1 |
| G: -6257.50192 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.35383 HOMO: -6.89537 LUMO: 2.12249 factor:1 | 1 (-0.48621) | -1 | -1 |
| G: -6257.50192 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.32243 HOMO: -6.28311 LUMO: 1.45037 factor:1 | 1 (-0.45481) | -1 | -1 |
| G: -6257.50192 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.53280 HOMO: -6.55522 LUMO: 1.39867 factor:1 | 1 (-0.66518) | -1 | -1 |
| G: -6257.50192 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.05756 HOMO: -6.46815 LUMO: 1.50207 factor:1 | -1 (0.81006) | -1 | -1 |
| G: -6257.50192 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.88541 HOMO: -6.43549 LUMO: 2.17419 factor:1 | 1 (-0.01780) | -1 | -1 |
| G: -6257.50192 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.32635 HOMO: -6.99333 LUMO: 1.87214 factor:1 | 1 (-0.45873) | -1 | -1 |
| G: -6257.50192 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.24403 HOMO: -6.65591 LUMO: 1.37962 factor:1 | 1 (-0.37642) | -1 | -1 |
| G: -6257.50192 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.87997 HOMO: -6.82734 LUMO: 1.55649 factor:1 | 1 (-0.01235) | -1 | -1 |
| G: -6257.50192 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.28175 HOMO: -6.71849 LUMO: 1.36057 factor:1 | 1 (-0.41413) | -1 | -1 |
| G: -6257.50192 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.11674 HOMO: -6.79468 LUMO: 1.82044 factor:1 | 1 (-0.24912) | -1 | -1 |
| G: -6257.50192 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.04018 HOMO: -6.61237 LUMO: 1.15104 factor:1 | 1 (-1.17257) | -1 | -1 |
| G: -6257.50192 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.16127 HOMO: -6.62053 LUMO: 2.33474 factor:1 | 1 (-1.29366) | -1 | -1 |
| G: -6257.50192 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.72077 HOMO: -6.55794 LUMO: 1.65717 factor:1 | 1 (-1.85315) | -1 | -1 |
| G: -6257.50192 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.81819 HOMO: -6.85999 LUMO: 2.03813 factor:1 | 1 (-0.95058) | -1 | -1 |
| G: -6257.50192 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.82965 HOMO: -6.45726 LUMO: 1.28438 factor:1 | 1 (-0.96203) | -1 | -1 |
| G: -6257.50192 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.30278 HOMO: -6.23685 LUMO: 1.93201 factor:1 | 1 (-0.43516) | -1 | -1 |
| G: -6257.50192 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.24343 HOMO: -7.06680 LUMO: 1.86942 factor:1 | 1 (-0.37582) | 1 | 1 |
| G: -6257.50192 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.78306 HOMO: -6.89537 LUMO: 2.17147 factor:1 | 1 (-0.91545) | -1 | -1 |
| G: -6257.50192 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.86010 HOMO: -6.80013 LUMO: 1.78779 factor:1 | 1 (-0.99248) | -1 | -1 |
| G: -6257.50192 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.23312 HOMO: -6.45726 LUMO: 1.58370 factor:1 | 1 (-0.36550) | -1 | -1 |
| G: -6257.50192 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.14795 HOMO: -6.52529 LUMO: 1.71976 factor:1 | 1 (-0.28033) | -1 | -1 |
| G: -6257.50192 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.77231 HOMO: -7.22462 LUMO: -1.18642 factor:1 | 1 (-0.90470) | 1 | 1 |
| G: -6257.50192 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.66224 HOMO: -7.18381 LUMO: -0.78641 factor:1 | 1 (-0.79463) | 1 | 1 |
| G: -6257.50192 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.18928 HOMO: -6.93346 LUMO: 1.65717 factor:1 | 1 (-0.32167) | -1 | -1 |
| G: -6257.50192 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.98846 HOMO: -6.41644 LUMO: 1.78235 factor:1 | 1 (-0.12085) | -1 | -1 |
| G: -6257.50192 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.41554 HOMO: -6.59876 LUMO: 1.83677 factor:1 | 1 (-1.54792) | -1 | -1 |
| G: -6257.50192 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12524.12137 HOMO: -6.35658 LUMO: 1.59731 factor:1 | 1 (-2.25376) | -1 | -1 |
| G: -6257.50192 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12524.18145 HOMO: -6.60692 LUMO: 1.66534 factor:1 | 1 (-2.31384) | -1 | -1 |
| G: -6257.50192 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.71144 HOMO: -6.83006 LUMO: 2.11705 factor:1 | 1 (-0.84383) | -1 | -1 |
| G: -6257.50192 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.17608 HOMO: -6.89264 LUMO: 1.30070 factor:1 | 1 (-0.30847) | -1 | -1 |
| G: -6257.50192 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.58991 HOMO: -6.90081 LUMO: 2.05174 factor:1 | 1 (-1.72229) | -1 | -1 |
| G: -6257.50192 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12524.07348 HOMO: -6.74842 LUMO: 1.96194 factor:1 | 1 (-2.20586) | -1 | -1 |
| G: -6257.50192 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.12386 HOMO: -6.58516 LUMO: 1.30887 factor:1 | 1 (-1.25624) | -1 | -1 |
| G: -6257.50192 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.86419 HOMO: -7.00965 LUMO: 2.08167 factor:1 | -1 (0.00343) | -1 | -1 |
| G: -6257.50192 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.18444 HOMO: -6.86815 LUMO: 2.29664 factor:1 | 1 (-0.31682) | -1 | -1 |
| G: -6257.50192 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.92998 HOMO: -6.39740 LUMO: 2.02725 factor:1 | 1 (-0.06237) | -1 | -1 |
| G: -6257.50192 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.53592 HOMO: -5.95929 LUMO: 1.62724 factor:1 | 1 (-1.66830) | -1 | -1 |
| G: -6257.50192 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.93919 HOMO: -6.71849 LUMO: 1.34696 factor:1 | 1 (-2.07158) | -1 | -1 |
| G: -6257.50192 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.12407 HOMO: -7.26816 LUMO: 1.74153 factor:1 | 1 (-1.25646) | 1 | 1 |
| G: -6257.50192 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.62643 HOMO: -6.90897 LUMO: 1.71432 factor:1 | 1 (-0.75882) | -1 | -1 |
| G: -6257.50192 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.82791 HOMO: -6.70489 LUMO: 1.91568 factor:1 | -1 (0.03970) | -1 | -1 |
| G: -6257.50192 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.06577 HOMO: -6.83278 LUMO: 1.61908 factor:1 | 1 (-0.19815) | -1 | -1 |
| G: -6257.50192 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.62962 HOMO: -7.17292 LUMO: 1.95378 factor:1 | 1 (-0.76200) | 1 | -1 |
| G: -6257.50192 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.88644 HOMO: -6.53345 LUMO: 1.74153 factor:1 | 1 (-1.01882) | -1 | -1 |
| G: -6257.50192 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.72240 HOMO: -6.53073 LUMO: 1.51023 factor:1 | 1 (-1.85478) | -1 | -1 |
| G: -6257.50192 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.58506 HOMO: -6.93346 LUMO: 2.22861 factor:1 | 1 (-1.71745) | -1 | -1 |
| G: -6257.50192 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.10503 HOMO: -6.47903 LUMO: 2.05446 factor:1 | 1 (-1.23741) | -1 | -1 |
| G: -6257.50192 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.55483 HOMO: -6.88992 LUMO: 1.57010 factor:1 | 1 (-1.68721) | -1 | -1 |
| G: -6257.50192 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.85531 HOMO: -6.07358 LUMO: 1.95922 factor:1 | 1 (-0.98769) | -1 | -1 |
| G: -6257.50192 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.88217 HOMO: -6.75114 LUMO: 2.18780 factor:1 | 1 (-1.01455) | -1 | -1 |
| G: -6257.50192 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.18350 HOMO: -6.96339 LUMO: 1.70071 factor:1 | 1 (-1.31589) | -1 | -1 |
| G: -6257.50192 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.32498 HOMO: -7.14843 LUMO: 1.82588 factor:1 | 1 (-0.45737) | 1 | -1 |
| G: -6257.50192 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.28673 HOMO: -6.96339 LUMO: 2.29392 factor:1 | -1 (0.58088) | -1 | -1 |
| G: -6257.50192 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.52709 HOMO: -6.81645 LUMO: 2.39732 factor:1 | -1 (0.34052) | -1 | -1 |
| G: -6257.50192 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12520.63118 HOMO: -6.48447 LUMO: 1.24084 factor:1 | -1 (1.23643) | -1 | -1 |
| G: -6257.50192 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.89485 HOMO: -7.14843 LUMO: 2.01092 factor:1 | 1 (-0.02724) | 1 | -1 |
| G: -6257.50192 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.78612 HOMO: -7.20013 LUMO: -0.34286 factor:1 | -1 (0.08150) | 1 | -1 |
| G: -6257.50192 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.24695 HOMO: -6.97700 LUMO: -0.15238 factor:1 | -1 (0.62066) | -1 | -1 |
| G: -6257.50192 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.45307 HOMO: -7.07768 LUMO: -0.26123 factor:1 | 1 (-0.58545) | 1 | -1 |
| G: -6257.50192 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.65634 HOMO: -6.99333 LUMO: -0.41361 factor:1 | 1 (-0.78872) | -1 | -1 |
| G: -6257.50192 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.08278 HOMO: -6.84638 LUMO: -0.40273 factor:1 | 1 (-0.21516) | -1 | -1 |
| G: -6257.50192 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.96465 HOMO: -6.83822 LUMO: -0.26939 factor:1 | 1 (-0.09704) | -1 | -1 |
| G: -6257.50192 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.97159 HOMO: -6.75931 LUMO: -0.93879 factor:1 | 1 (-0.10397) | -1 | -1 |
| G: -6257.50192 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.95023 HOMO: -6.79468 LUMO: -0.39729 factor:1 | 1 (-0.08261) | -1 | -1 |
| G: -6257.50192 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.59009 HOMO: -6.93890 LUMO: 0.43266 factor:1 | -1 (0.27753) | -1 | -1 |
| G: -6257.50192 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.69554 HOMO: -7.08040 LUMO: -0.85716 factor:1 | 1 (-1.82792) | 1 | 1 |
| G: -6257.50192 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.87419 HOMO: -6.70216 LUMO: -1.41499 factor:1 | 1 (-1.00658) | -1 | -1 |
| G: -6257.50192 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.80918 HOMO: -6.63686 LUMO: -0.52790 factor:1 | 1 (-0.94157) | -1 | -1 |
| G: -6257.50192 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.71264 HOMO: -6.75114 LUMO: -0.13334 factor:1 | 1 (-0.84502) | -1 | -1 |
| G: -6257.50192 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.03058 HOMO: -6.94435 LUMO: -0.24490 factor:1 | 1 (-1.16296) | -1 | -1 |
| G: -6257.50192 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.43988 HOMO: -6.74298 LUMO: -0.84627 factor:1 | -1 (0.42774) | -1 | -1 |
| G: -6257.50192 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.73931 HOMO: -7.15932 LUMO: 0.22041 factor:1 | 1 (-0.87169) | 1 | 1 |
| G: -6257.50192 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.48597 HOMO: -6.90081 LUMO: -1.16737 factor:1 | 1 (-0.61835) | -1 | -1 |
| G: -6257.50192 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.98628 HOMO: -7.04775 LUMO: -0.84355 factor:1 | 1 (-0.11867) | -1 | -1 |
| G: -6257.50192 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.89610 HOMO: -7.17020 LUMO: -1.31159 factor:1 | 1 (-1.02848) | 1 | 1 |
| G: -6257.50192 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.74633 HOMO: -7.14571 LUMO: -0.46259 factor:1 | 1 (-0.87871) | 1 | 1 |
| G: -6257.50192 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.99940 HOMO: -7.45048 LUMO: -0.91158 factor:1 | 1 (-0.13178) | 1 | 1 |
| G: -6257.50192 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.57248 HOMO: -6.87360 LUMO: -0.82995 factor:1 | -1 (0.29513) | -1 | -1 |
| G: -6257.50192 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.56516 HOMO: -7.43415 LUMO: -0.65307 factor:1 | -1 (0.30245) | 1 | 1 |
| G: -6257.50192 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.76350 HOMO: -7.47225 LUMO: -0.77280 factor:1 | 1 (-0.89588) | 1 | 1 |
| G: -6257.50192 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.67699 HOMO: -6.86271 LUMO: -0.83811 factor:1 | 1 (-0.80938) | -1 | -1 |
| G: -6257.50192 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.22275 HOMO: -7.53483 LUMO: -0.66124 factor:1 | 1 (-0.35514) | 1 | 1 |
| G: -6257.50192 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.65946 HOMO: -7.45864 LUMO: -1.08301 factor:1 | 1 (-1.79184) | 1 | 1 |
| G: -6257.50192 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12524.04738 HOMO: -7.24639 LUMO: -1.19186 factor:1 | 1 (-2.17977) | 1 | 1 |
| G: -6257.50192 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.16342 HOMO: -7.54844 LUMO: -0.96873 factor:1 | 1 (-1.29581) | 1 | 1 |
| G: -6257.50192 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.90148 HOMO: -7.12666 LUMO: -0.01633 factor:1 | 1 (-2.03386) | 1 | 1 |
| G: -6257.50192 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.00176 HOMO: -6.77291 LUMO: -0.70477 factor:1 | 1 (-1.13414) | -1 | -1 |
| G: -6257.50192 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.17567 HOMO: -6.76475 LUMO: -1.15921 factor:1 | 1 (-1.30805) | -1 | -1 |
| G: -6257.50192 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.91833 HOMO: -5.37697 LUMO: -0.56600 factor:1 | 1 (-1.05071) | -1 | -1 |
| G: -6257.50192 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.42191 HOMO: -6.62053 LUMO: -1.75513 factor:1 | 1 (-0.55430) | -1 | -1 |
| G: -6257.50192 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.70951 HOMO: -6.60420 LUMO: -1.74697 factor:1 | 1 (-0.84189) | -1 | -1 |
| G: -6257.50192 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.46575 HOMO: -6.84366 LUMO: -0.94968 factor:1 | 1 (-0.59813) | -1 | -1 |
| G: -6257.50192 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.39972 HOMO: -6.96884 LUMO: -2.11977 factor:1 | -1 (0.46790) | -1 | -1 |
| G: -6257.50192 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.33942 HOMO: -6.80829 LUMO: 0.56055 factor:1 | -1 (0.52820) | -1 | -1 |
| G: -6257.50192 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.94108 HOMO: -7.02326 LUMO: 0.11429 factor:1 | 1 (-1.07346) | -1 | -1 |
| G: -6257.50192 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.06747 HOMO: -7.40966 LUMO: 0.18232 factor:1 | 1 (-1.19986) | 1 | 1 |
| G: -6257.50192 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.29334 HOMO: -6.34570 LUMO: 0.41089 factor:1 | 1 (-0.42572) | -1 | -1 |
| G: -6257.50192 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.11418 HOMO: -6.78924 LUMO: 0.49525 factor:1 | 1 (-0.24656) | -1 | -1 |
| G: -6257.50192 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.87190 HOMO: -6.87632 LUMO: 0.44082 factor:1 | 1 (-2.00428) | -1 | -1 |
| G: -6257.50192 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12524.25231 HOMO: -6.69944 LUMO: 1.20546 factor:1 | 1 (-2.38470) | -1 | -1 |
| G: -6257.50192 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.74561 HOMO: -6.83006 LUMO: 1.28982 factor:1 | 1 (-1.87799) | -1 | -1 |
| G: -6257.50192 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12524.04194 HOMO: -7.78246 LUMO: 0.20681 factor:1 | 1 (-2.17433) | 1 | 1 |
| G: -6257.50192 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.94232 HOMO: -6.55794 LUMO: -1.65173 factor:1 | 1 (-2.07470) | -1 | -1 |
| G: -6257.50192 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.23186 HOMO: -6.77564 LUMO: -1.14560 factor:1 | 1 (-1.36424) | -1 | -1 |
| G: -6257.50192 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.06327 HOMO: -7.46680 LUMO: -1.18097 factor:1 | 1 (-0.19565) | 1 | 1 |
| G: -6257.50192 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.88548 HOMO: -6.88176 LUMO: -1.24900 factor:1 | 1 (-1.01787) | -1 | -1 |
| G: -6257.50192 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.90157 HOMO: -7.28177 LUMO: -0.42178 factor:1 | 1 (-1.03395) | 1 | 1 |
| G: -6257.50192 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.85052 HOMO: -7.71715 LUMO: 0.19592 factor:1 | 1 (-0.98290) | 1 | 1 |
| G: -6257.50192 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.16980 HOMO: -7.02326 LUMO: -1.40683 factor:1 | 1 (-0.30218) | -1 | -1 |
| G: -6257.50192 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.73492 HOMO: -7.27088 LUMO: -1.07485 factor:1 | 1 (-1.86730) | 1 | 1 |
| G: -6257.50192 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.66286 HOMO: -7.17020 LUMO: -0.49525 factor:1 | 1 (-1.79524) | 1 | 1 |
| G: -6257.50192 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.10824 HOMO: -7.15932 LUMO: 0.02721 factor:1 | 1 (-1.24062) | 1 | 1 |
| G: -6257.50192 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.86836 HOMO: -7.00693 LUMO: -0.83267 factor:1 | 1 (-2.00074) | -1 | -1 |
| G: -6257.50192 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.13763 HOMO: -6.86543 LUMO: -0.10340 factor:1 | 1 (-1.27001) | -1 | -1 |
| G: -6257.50192 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.14179 HOMO: -7.11850 LUMO: -0.08980 factor:1 | 1 (-1.27417) | 1 | 1 |
| G: -6257.50192 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.27560 HOMO: -6.87087 LUMO: -0.88981 factor:1 | -1 (0.59201) | -1 | -1 |
| G: -6257.50192 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.27626 HOMO: -7.08857 LUMO: -1.27077 factor:1 | -1 (0.59136) | 1 | 1 |
| G: -6257.50192 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.95837 HOMO: -6.79468 LUMO: -0.81906 factor:1 | 1 (-0.09075) | -1 | -1 |
| G: -6257.50192 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.04563 HOMO: -6.86815 LUMO: -0.89798 factor:1 | 1 (-0.17802) | -1 | -1 |
| G: -6257.50192 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.92528 HOMO: -6.78652 LUMO: -2.00548 factor:1 | 1 (-0.05766) | -1 | -1 |
| G: -6257.50192 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.04637 HOMO: -6.75114 LUMO: -0.08436 factor:1 | 1 (-0.17875) | -1 | -1 |
| G: -6257.50192 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.12026 HOMO: -6.55794 LUMO: 0.52790 factor:1 | -1 (0.74736) | -1 | -1 |
| G: -6257.50192 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.91057 HOMO: -7.17836 LUMO: 0.28300 factor:1 | 1 (-1.04296) | 1 | -1 |
| G: -6257.50192 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.04592 HOMO: -7.35796 LUMO: -0.77552 factor:1 | 1 (-1.17831) | 1 | 1 |
| G: -6257.50192 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.80289 HOMO: -7.23551 LUMO: -1.17553 factor:1 | 1 (-1.93527) | 1 | 1 |
| G: -6257.50192 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.33151 HOMO: -7.07496 LUMO: -1.14288 factor:1 | 1 (-1.46389) | 1 | 1 |
| G: -6257.50192 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.96486 HOMO: -6.70489 LUMO: -0.83539 factor:1 | 1 (-1.09724) | -1 | -1 |
| G: -6257.50192 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.19051 HOMO: -6.59604 LUMO: -0.89798 factor:1 | -1 (0.67710) | -1 | -1 |
| G: -6257.50192 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.05797 HOMO: -6.94162 LUMO: -1.22451 factor:1 | -1 (0.80965) | -1 | -1 |
| G: -6257.50192 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.88272 HOMO: -6.68040 LUMO: 0.22041 factor:1 | 1 (-0.01510) | -1 | -1 |
| G: -6257.50192 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.83033 HOMO: -6.88176 LUMO: 0.11157 factor:1 | 1 (-0.96271) | -1 | -1 |
| G: -6257.50192 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.59762 HOMO: -6.91713 LUMO: 1.27621 factor:1 | 1 (-0.73000) | -1 | -1 |
| G: -6257.50192 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.14974 HOMO: -6.77836 LUMO: 1.01226 factor:1 | 1 (-0.28213) | -1 | -1 |
| G: -6257.50192 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.91085 HOMO: -7.14571 LUMO: 1.48574 factor:1 | 1 (-1.04323) | 1 | 1 |
| G: -6257.50192 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.86704 HOMO: -6.96884 LUMO: 1.48574 factor:1 | -1 (0.00057) | -1 | -1 |
| G: -6257.50192 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.00095 HOMO: -7.24367 LUMO: 1.28438 factor:1 | 1 (-0.13334) | 1 | 1 |
| G: -6257.50192 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.83235 HOMO: -7.10489 LUMO: 1.29526 factor:1 | -1 (0.03527) | 1 | 1 |
| G: -6257.50192 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.68967 HOMO: -7.07224 LUMO: 1.29254 factor:1 | 1 (-0.82206) | 1 | 1 |
| G: -6257.50192 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.95056 HOMO: -7.12938 LUMO: 0.49253 factor:1 | 1 (-0.08294) | 1 | 1 |
| G: -6257.50192 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.69740 HOMO: -7.33619 LUMO: 1.45581 factor:1 | 1 (-0.82978) | 1 | 1 |
| G: -6257.50192 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.97839 HOMO: -6.87904 LUMO: -0.14422 factor:1 | 1 (-0.11078) | -1 | -1 |
| G: -6257.50192 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.94206 HOMO: -6.81917 LUMO: 0.50341 factor:1 | 1 (-1.07444) | -1 | -1 |
| G: -6257.50192 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.72603 HOMO: -7.27905 LUMO: 0.13606 factor:1 | 1 (-0.85841) | 1 | -1 |
| G: -6257.50192 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.84323 HOMO: -6.87904 LUMO: -0.09796 factor:1 | 1 (-0.97561) | -1 | -1 |
| G: -6257.50192 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.93961 HOMO: -7.33891 LUMO: 0.03810 factor:1 | 1 (-1.07199) | 1 | 1 |
| G: -6257.50192 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.02211 HOMO: -6.98516 LUMO: 0.98233 factor:1 | 1 (-1.15450) | -1 | -1 |
| G: -6257.50192 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.07052 HOMO: -6.94162 LUMO: 0.86804 factor:1 | 1 (-1.20291) | -1 | -1 |
| G: -6257.50192 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.15114 HOMO: -7.37701 LUMO: 0.05442 factor:1 | -1 (0.71648) | 1 | 1 |
| G: -6257.50192 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.07850 HOMO: -7.04775 LUMO: 0.43266 factor:1 | 1 (-0.21089) | -1 | -1 |
| G: -6257.50192 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.98552 HOMO: -7.47497 LUMO: 0.31837 factor:1 | 1 (-0.11791) | 1 | 1 |
| G: -6257.50192 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.84100 HOMO: -6.62053 LUMO: 0.13061 factor:1 | -1 (0.02661) | -1 | -1 |
| G: -6257.50192 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.58737 HOMO: -6.44366 LUMO: -0.04354 factor:1 | -1 (0.28025) | -1 | -1 |
| G: -6257.50192 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.06767 HOMO: -6.40284 LUMO: 0.68301 factor:1 | 1 (-0.20006) | -1 | -1 |
| G: -6257.50192 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.05739 HOMO: -6.73754 LUMO: 0.36735 factor:1 | 1 (-0.18977) | -1 | -1 |
| G: -6257.50192 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.04582 HOMO: -6.85455 LUMO: 0.23946 factor:1 | 1 (-0.17821) | -1 | -1 |
| G: -6257.50192 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.92707 HOMO: -6.93346 LUMO: 0.24762 factor:1 | 1 (-0.05946) | -1 | -1 |
| G: -6257.50192 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.90917 HOMO: -6.85455 LUMO: 0.17687 factor:1 | 1 (-0.04155) | -1 | -1 |
| G: -6257.50192 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.71572 HOMO: -6.62325 LUMO: 0.69933 factor:1 | -1 (0.15189) | -1 | -1 |
| G: -6257.50192 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.91744 HOMO: -6.43005 LUMO: 0.50069 factor:1 | 1 (-0.04982) | -1 | -1 |
| G: -6257.50192 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.83841 HOMO: -6.56883 LUMO: 0.22858 factor:1 | 1 (-0.97079) | -1 | -1 |
| G: -6257.50192 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.76769 HOMO: -6.78380 LUMO: 0.54967 factor:1 | 1 (-0.90007) | -1 | -1 |
| G: -6257.50192 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.84233 HOMO: -7.35524 LUMO: 0.00272 factor:1 | 1 (-0.97471) | 1 | 1 |
| G: -6257.50192 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.54853 HOMO: -7.27360 LUMO: 0.08436 factor:1 | 1 (-0.68091) | 1 | 1 |
| G: -6257.50192 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.87030 HOMO: -7.44504 LUMO: -0.96056 factor:1 | 1 (-1.00269) | 1 | 1 |
| G: -6257.50192 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.74722 HOMO: -7.27360 LUMO: 0.29933 factor:1 | 1 (-0.87961) | 1 | 1 |
| G: -6257.50192 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.68635 HOMO: -7.09129 LUMO: 0.41089 factor:1 | 1 (-0.81874) | 1 | 1 |
| G: -6257.50192 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.80924 HOMO: -6.93618 LUMO: 0.36463 factor:1 | 1 (-0.94162) | -1 | -1 |
| G: -6257.50192 HOMO: -7.26000 LUMO: -3.02863 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.19154 HOMO: -7.65728 LUMO: 0.20136 factor:1 | 1 (-0.32392) | 1 | 1 |
| G: -6257.50192 HOMO: -7.26000 LUMO: -3.02863 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.32379 HOMO: -6.90353 LUMO: -0.92791 factor:1 | 1 (-0.45617) | -1 | -1 |
| G: -6257.50192 HOMO: -7.26000 LUMO: -3.02863 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.03741 HOMO: -6.82462 LUMO: -1.18370 factor:1 | 1 (-0.16980) | -1 | -1 |
| G: -6257.50192 HOMO: -7.26000 LUMO: -3.02863 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.01880 HOMO: -7.09129 LUMO: -0.13334 factor:1 | 1 (-0.15119) | 1 | 1 |
| G: -6257.50192 HOMO: -7.26000 LUMO: -3.02863 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.06411 HOMO: -7.40966 LUMO: -1.06941 factor:1 | 1 (-0.19649) | 1 | 1 |
| G: -6257.50192 HOMO: -7.26000 LUMO: -3.02863 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.99815 HOMO: -7.24367 LUMO: -1.00954 factor:1 | 1 (-0.13053) | 1 | 1 |
| G: -6257.50192 HOMO: -7.26000 LUMO: -3.02863 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.97001 HOMO: -7.51851 LUMO: 0.09796 factor:1 | 1 (-0.10240) | 1 | 1 |
| G: -6257.50192 HOMO: -7.26000 LUMO: -3.02863 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.72480 HOMO: -7.48857 LUMO: -0.07619 factor:1 | 1 (-0.85719) | 1 | 1 |
| G: -6257.50192 HOMO: -7.26000 LUMO: -3.02863 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.65484 HOMO: -6.53345 LUMO: 1.09390 factor:1 | 1 (-0.78723) | -1 | -1 |
| G: -6257.50192 HOMO: -7.26000 LUMO: -3.02863 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.96954 HOMO: -7.21918 LUMO: 0.08436 factor:1 | 1 (-1.10193) | 1 | 1 |
| G: -6257.50192 HOMO: -7.26000 LUMO: -3.02863 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.55555 HOMO: -7.38789 LUMO: 1.02587 factor:1 | 1 (-0.68793) | 1 | -1 |
| G: -6257.50192 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.68989 HOMO: -6.83550 LUMO: -0.67484 factor:1 | 1 (-0.82227) | -1 | -1 |
| G: -6257.50192 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.80943 HOMO: -7.04231 LUMO: 0.54151 factor:1 | 1 (-0.94181) | -1 | -1 |
| G: -6257.50192 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.98316 HOMO: -6.79740 LUMO: 1.91296 factor:1 | 1 (-2.11555) | 1 | 1 |
| G: -6257.50192 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.30895 HOMO: -7.35796 LUMO: -1.04220 factor:1 | 1 (-1.44133) | -1 | -1 |
| G: -6257.50192 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.52269 HOMO: -6.62597 LUMO: -0.44082 factor:1 | 1 (-1.65508) | -1 | -1 |
| G: -6257.50192 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.98814 HOMO: -6.45182 LUMO: -0.20409 factor:1 | 1 (-2.12053) | -1 | -1 |
| G: -6257.50192 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.82132 HOMO: -6.51168 LUMO: -0.23130 factor:1 | 1 (-0.95370) | -1 | -1 |
| G: -6257.50192 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.43718 HOMO: -7.14027 LUMO: 0.49797 factor:1 | 1 (-0.56956) | -1 | -1 |
| G: -6257.50192 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.57933 HOMO: -7.55660 LUMO: 0.24762 factor:1 | 1 (-0.71171) | -1 | -1 |
| G: -6257.50192 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.67517 HOMO: -6.88992 LUMO: -0.64763 factor:1 | 1 (-0.80755) | -1 | -1 |
| G: -6257.50192 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.16823 HOMO: -6.72665 LUMO: -0.45987 factor:1 | -1 (0.69939) | -1 | -1 |
| G: -6257.50192 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.15963 HOMO: -6.72121 LUMO: -0.58232 factor:1 | -1 (0.70799) | -1 | -1 |
| G: -6257.50192 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.74018 HOMO: -7.26816 LUMO: 0.32926 factor:1 | 1 (-0.87256) | -1 | -1 |
| G: -6257.50192 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.66499 HOMO: -6.57155 LUMO: -0.53606 factor:1 | 1 (-0.79738) | -1 | -1 |
| G: -6257.50192 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.88521 HOMO: -6.50896 LUMO: -0.43810 factor:1 | 1 (-1.01760) | -1 | -1 |
| G: -6257.50192 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.38080 HOMO: -6.73210 LUMO: -0.51430 factor:1 | 1 (-0.51318) | -1 | -1 |
| G: -6257.50192 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.33070 HOMO: -6.77019 LUMO: -0.62858 factor:1 | 1 (-0.46308) | -1 | -1 |
| G: -6257.50192 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.35263 HOMO: -6.82462 LUMO: -0.67484 factor:1 | 1 (-0.48502) | -1 | -1 |
| G: -6257.50192 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.78962 HOMO: -6.79740 LUMO: -0.55511 factor:1 | 1 (-0.92200) | -1 | -1 |
| G: -6257.50192 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.18573 HOMO: -6.79740 LUMO: -0.67756 factor:1 | -1 (0.68189) | -1 | -1 |
| G: -6257.50192 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.21196 HOMO: -6.75114 LUMO: -0.55239 factor:1 | -1 (0.65566) | -1 | -1 |
| G: -6257.50192 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.37697 HOMO: -6.49536 LUMO: -0.25307 factor:1 | -1 (0.49065) | -1 | -1 |
| G: -6257.50192 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.11138 HOMO: -6.48992 LUMO: -0.25034 factor:1 | 1 (-0.24376) | -1 | -1 |
| G: -6257.50192 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.76690 HOMO: -6.52801 LUMO: -0.28028 factor:1 | 1 (-0.89928) | -1 | -1 |
| G: -6257.50192 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.30251 HOMO: -7.22462 LUMO: 0.52518 factor:1 | 1 (-0.43489) | -1 | -1 |
| G: -6257.50192 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.30178 HOMO: -6.59332 LUMO: -0.27211 factor:1 | -1 (0.56583) | -1 | -1 |
| G: -6257.50192 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.30872 HOMO: -6.57427 LUMO: -0.16871 factor:1 | -1 (0.55889) | -1 | -1 |
| G: -6257.50192 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.26336 HOMO: -6.71033 LUMO: 1.59187 factor:1 | -1 (0.60426) | 1 | 1 |
| G: -6257.50192 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.11650 HOMO: -6.72121 LUMO: 2.00004 factor:1 | -1 (0.75112) | 1 | 1 |
| G: -6257.50192 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.17032 HOMO: -6.61509 LUMO: 1.55921 factor:1 | -1 (0.69729) | -1 | -1 |
| G: -6257.50192 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.33808 HOMO: -6.55250 LUMO: 1.73064 factor:1 | -1 (0.52953) | -1 | -1 |
| G: -6257.50192 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.88060 HOMO: -6.66135 LUMO: 2.02181 factor:1 | 1 (-0.01298) | 1 | 1 |
| G: -6257.50192 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.86212 HOMO: -6.84911 LUMO: 1.98099 factor:1 | -1 (0.00550) | 1 | 1 |
| G: -6257.50192 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.79700 HOMO: -6.66679 LUMO: 1.98371 factor:1 | -1 (0.07061) | 1 | 1 |
| G: -6257.50192 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.37876 HOMO: -6.67495 LUMO: 2.04085 factor:1 | -1 (0.48885) | 1 | 1 |
| G: -6257.50192 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.16809 HOMO: -6.89809 LUMO: 1.95106 factor:1 | -1 (0.69952) | 1 | 1 |
| G: -6257.50192 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.09038 HOMO: -6.50352 LUMO: 1.88847 factor:1 | -1 (0.77724) | -1 | -1 |
| G: -6257.50192 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.00556 HOMO: -6.93618 LUMO: 2.00004 factor:1 | -1 (0.86206) | 1 | 1 |
| G: -6257.50192 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.45647 HOMO: -6.50896 LUMO: 1.73609 factor:1 | 1 (-0.58885) | -1 | -1 |
| G: -6257.50192 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.10231 HOMO: -6.69672 LUMO: 2.37283 factor:1 | 1 (-1.23469) | 1 | 1 |
| G: -6257.50192 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.06923 HOMO: -6.65591 LUMO: 2.20684 factor:1 | -1 (0.79838) | 1 | 1 |
| G: -6257.50192 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12520.89309 HOMO: -6.23957 LUMO: 1.78507 factor:1 | -1 (0.97452) | -1 | -1 |
| G: -6257.50192 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.66028 HOMO: -6.35114 LUMO: 1.92112 factor:1 | 1 (-0.79267) | -1 | -1 |
| G: -6257.50192 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.84772 HOMO: -6.53617 LUMO: 1.75241 factor:1 | -1 (0.01989) | -1 | -1 |
| G: -6257.50192 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.05937 HOMO: -6.60420 LUMO: 1.78779 factor:1 | 1 (-0.19176) | 1 | 1 |
| G: -6257.50192 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.68519 HOMO: -7.40422 LUMO: -0.97145 factor:1 | -1 (0.18243) | -1 | -1 |
| G: -6257.50192 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.78027 HOMO: -6.80013 LUMO: -0.69117 factor:1 | -1 (0.08735) | -1 | -1 |
| G: -6257.50192 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.45406 HOMO: -6.68040 LUMO: -0.47076 factor:1 | -1 (0.41356) | -1 | -1 |
| G: -6257.50192 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.38997 HOMO: -7.20285 LUMO: -0.66124 factor:1 | -1 (0.47764) | -1 | -1 |
| G: -6257.50192 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.49702 HOMO: -6.82734 LUMO: -0.60137 factor:1 | -1 (0.37059) | -1 | -1 |
| G: -6257.50192 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.43969 HOMO: -7.18653 LUMO: 0.59321 factor:1 | -1 (0.42793) | -1 | -1 |
| G: -6257.50192 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.50214 HOMO: -7.29265 LUMO: 0.48164 factor:1 | -1 (0.36548) | -1 | -1 |
| G: -6257.50192 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.59226 HOMO: -6.63414 LUMO: -0.25034 factor:1 | -1 (0.27535) | -1 | -1 |
| G: -6257.50192 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.53915 HOMO: -7.20285 LUMO: 0.53879 factor:1 | -1 (0.32847) | -1 | -1 |
| G: -6257.50192 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.53945 HOMO: -6.46815 LUMO: -0.21769 factor:1 | -1 (0.32817) | -1 | -1 |
| G: -6257.50192 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.63368 HOMO: -6.57971 LUMO: -0.18776 factor:1 | -1 (0.23394) | -1 | -1 |
| G: -6257.50192 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.62763 HOMO: -6.90897 LUMO: 1.91296 factor:1 | 1 (-0.76001) | 1 | 1 |
| G: -6257.50192 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.70271 HOMO: -6.67495 LUMO: 2.04358 factor:1 | 1 (-0.83509) | 1 | 1 |
| G: -6257.50192 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.73218 HOMO: -6.94162 LUMO: 1.73881 factor:1 | 1 (-0.86456) | 1 | 1 |
| G: -6257.50192 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.54053 HOMO: -6.73482 LUMO: 1.95922 factor:1 | 1 (-0.67291) | 1 | 1 |
| G: -6257.50192 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.14370 HOMO: -6.70489 LUMO: 2.04358 factor:1 | 1 (-0.27609) | 1 | 1 |
| G: -6257.50192 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.22569 HOMO: -7.04231 LUMO: 1.79323 factor:1 | 1 (-0.35807) | 1 | 1 |
| G: -6257.50192 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.12071 HOMO: -6.68584 LUMO: 1.60275 factor:1 | 1 (-0.25309) | 1 | 1 |
| G: -6257.50192 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.20355 HOMO: -6.40556 LUMO: 1.45581 factor:1 | -1 (0.66407) | -1 | -1 |
| G: -6257.50192 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.44379 HOMO: -6.94979 LUMO: 2.16603 factor:1 | 1 (-0.57617) | 1 | 1 |
| G: -6257.50192 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.60115 HOMO: -6.84911 LUMO: 1.89935 factor:1 | 1 (-0.73354) | 1 | 1 |
| G: -6257.50192 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.71193 HOMO: -6.22052 LUMO: 1.57282 factor:1 | 1 (-0.84431) | -1 | -1 |
| G: -6257.50192 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.22368 HOMO: -6.51168 LUMO: 2.10072 factor:1 | 1 (-0.35606) | -1 | -1 |
| G: -6257.50192 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.78448 HOMO: -7.03686 LUMO: 2.12249 factor:1 | 1 (-0.91686) | 1 | 1 |
| G: -6257.50192 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.44453 HOMO: -6.84094 LUMO: 1.63268 factor:1 | -1 (0.42308) | 1 | 1 |
| G: -6257.50192 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.49335 HOMO: -6.75387 LUMO: 1.72248 factor:1 | -1 (0.37427) | 1 | 1 |
| G: -6257.50192 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.39999 HOMO: -6.86271 LUMO: 1.68711 factor:1 | -1 (0.46763) | 1 | 1 |
| G: -6257.50192 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.42894 HOMO: -6.84094 LUMO: 2.02997 factor:1 | -1 (0.43867) | 1 | 1 |
| G: -6257.50192 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.40864 HOMO: -6.80557 LUMO: 2.02725 factor:1 | -1 (0.45897) | 1 | 1 |
| G: -6257.50192 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.19370 HOMO: -6.38651 LUMO: 1.53472 factor:1 | -1 (0.67392) | -1 | -1 |
| G: -6257.50192 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.12243 HOMO: -7.51306 LUMO: 0.28572 factor:1 | -1 (0.74518) | -1 | -1 |
| G: -6257.50192 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.08643 HOMO: -6.97972 LUMO: -0.74287 factor:1 | -1 (0.78118) | -1 | -1 |
| G: -6257.50192 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.96786 HOMO: -6.83822 LUMO: -0.65852 factor:1 | 1 (-0.10025) | -1 | -1 |
| G: -6257.50192 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.06433 HOMO: -6.71305 LUMO: -0.49525 factor:1 | 1 (-0.19671) | -1 | -1 |
| G: -6257.50192 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.54873 HOMO: -6.60692 LUMO: -0.22313 factor:1 | -1 (0.31889) | -1 | -1 |
| G: -6257.50192 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.75621 HOMO: -7.20013 LUMO: 0.55239 factor:1 | -1 (0.11140) | -1 | -1 |
| G: -6257.50192 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.00822 HOMO: -6.60420 LUMO: -0.28028 factor:1 | 1 (-0.14060) | -1 | -1 |
| G: -6257.50192 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.02735 HOMO: -6.69128 LUMO: -0.30477 factor:1 | 1 (-0.15973) | -1 | -1 |
| G: -6257.50192 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.00718 HOMO: -6.65591 LUMO: -0.25579 factor:1 | 1 (-0.13957) | -1 | -1 |
| G: -6257.50192 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.00778 HOMO: -6.69128 LUMO: 1.70888 factor:1 | 1 (-0.14017) | 1 | 1 |
| G: -6257.50192 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.05935 HOMO: -6.50080 LUMO: 1.87759 factor:1 | 1 (-0.19173) | -1 | -1 |
| G: -6257.50192 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.49779 HOMO: -6.85727 LUMO: 1.99187 factor:1 | -1 (0.36983) | 1 | 1 |
| G: -6257.50192 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.76473 HOMO: -6.58788 LUMO: 1.79051 factor:1 | -1 (0.10289) | 1 | 1 |
| G: -6257.50192 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.49057 HOMO: -6.64230 LUMO: 2.16058 factor:1 | -1 (0.37704) | 1 | 1 |
| G: -6257.50192 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.43202 HOMO: -6.58788 LUMO: 2.10616 factor:1 | -1 (0.43560) | 1 | 1 |
| G: -6257.50192 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.43768 HOMO: -7.01782 LUMO: 2.13609 factor:1 | -1 (0.42994) | 1 | 1 |
| G: -6257.50192 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.06463 HOMO: -6.31304 LUMO: 2.31841 factor:1 | -1 (0.80298) | -1 | -1 |
| G: -6257.50192 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12520.81481 HOMO: -6.94979 LUMO: 2.07895 factor:1 | -1 (1.05281) | 1 | 1 |
| G: -6257.50192 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12520.80771 HOMO: -6.88992 LUMO: 2.28031 factor:1 | -1 (1.05991) | 1 | 1 |
| G: -6257.50192 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.96950 HOMO: -6.66407 LUMO: 2.07623 factor:1 | 1 (-0.10188) | 1 | 1 |
| G: -6257.50192 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.08335 HOMO: -6.52529 LUMO: 1.70071 factor:1 | 1 (-0.21573) | -1 | -1 |
| G: -6257.50192 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.17535 HOMO: -6.58788 LUMO: 1.57282 factor:1 | 1 (-0.30773) | -1 | -1 |
| G: -6257.50192 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.33207 HOMO: -6.55250 LUMO: 1.95378 factor:1 | -1 (0.53555) | -1 | -1 |
| G: -6257.50192 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.49011 HOMO: -6.24773 LUMO: 1.77962 factor:1 | -1 (0.37750) | -1 | -1 |
| G: -6257.50192 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.51175 HOMO: -6.31304 LUMO: 2.18507 factor:1 | -1 (0.35587) | -1 | -1 |
| G: -6257.50192 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.99322 HOMO: -6.18243 LUMO: 2.01636 factor:1 | 1 (-0.12561) | -1 | -1 |
| G: -6257.50192 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.28586 HOMO: -6.99877 LUMO: 2.14970 factor:1 | -1 (0.58175) | 1 | 1 |
| G: -6257.50192 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.58554 HOMO: -6.72665 LUMO: 2.07079 factor:1 | -1 (0.28207) | 1 | 1 |
| G: -6257.50192 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.01799 HOMO: -6.36202 LUMO: 2.17419 factor:1 | 1 (-0.15037) | -1 | -1 |
| G: -6257.50192 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.07127 HOMO: -6.78652 LUMO: 2.05718 factor:1 | 1 (-0.20365) | 1 | -1 |
| G: -6257.50192 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.14563 HOMO: -6.87360 LUMO: 2.34290 factor:1 | 1 (-0.27802) | 1 | 1 |
| G: -6257.50192 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.05556 HOMO: -6.62053 LUMO: 1.89391 factor:1 | 1 (-0.18795) | 1 | 1 |
| G: -6257.50192 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.30395 HOMO: -6.58788 LUMO: 1.83133 factor:1 | 1 (-0.43633) | 1 | 1 |
| G: -6257.50192 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.62168 HOMO: -7.08584 LUMO: 1.91568 factor:1 | -1 (0.24594) | 1 | 1 |
| G: -6257.50192 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.96003 HOMO: -6.56883 LUMO: 1.81228 factor:1 | 1 (-0.09241) | 1 | 1 |
| G: -6257.50192 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.01061 HOMO: -6.66135 LUMO: 1.92384 factor:1 | 1 (-0.14300) | 1 | 1 |
| G: -6257.50192 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.08098 HOMO: -6.64502 LUMO: 2.15786 factor:1 | 1 (-0.21336) | 1 | 1 |
| G: -6257.50192 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.21965 HOMO: -6.71305 LUMO: 1.91840 factor:1 | 1 (-0.35203) | 1 | 1 |
| G: -6257.50192 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.85698 HOMO: -6.44094 LUMO: 1.74425 factor:1 | -1 (0.01064) | -1 | -1 |
| G: -6257.50192 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.10721 HOMO: -6.51985 LUMO: 1.84221 factor:1 | 1 (-0.23960) | -1 | -1 |
| G: -6257.50192 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.92321 HOMO: -6.63414 LUMO: -0.24762 factor:1 | 1 (-0.05559) | -1 | -1 |
| G: -6257.50192 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.05524 HOMO: -6.60420 LUMO: -0.22585 factor:1 | 1 (-0.18762) | -1 | -1 |
| G: -6257.50192 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.15789 HOMO: -7.19741 LUMO: 0.58232 factor:1 | -1 (0.70973) | -1 | -1 |
| G: -6257.50192 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12520.94518 HOMO: -6.77019 LUMO: -0.56872 factor:1 | -1 (0.92244) | -1 | -1 |
| G: -6257.50192 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.04824 HOMO: -7.46136 LUMO: 0.28844 factor:1 | 1 (-0.18063) | -1 | -1 |
| G: -6257.50192 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.02740 HOMO: -6.60420 LUMO: -0.54151 factor:1 | 1 (-0.15979) | -1 | -1 |
| G: -6257.50192 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.04672 HOMO: -6.53890 LUMO: -0.46531 factor:1 | 1 (-0.17911) | -1 | -1 |
| G: -6257.50192 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.00337 HOMO: -6.81645 LUMO: -0.57144 factor:1 | 1 (-0.13576) | -1 | -1 |
| G: -6257.50192 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.03094 HOMO: -7.48041 LUMO: 0.28572 factor:1 | 1 (-0.16332) | -1 | -1 |
| G: -6257.50192 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.03967 HOMO: -6.75659 LUMO: -0.45715 factor:1 | 1 (-0.17206) | -1 | -1 |
| G: -6257.50192 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.73039 HOMO: -6.66135 LUMO: -0.41906 factor:1 | -1 (0.13723) | -1 | -1 |
| G: -6257.50192 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.66603 HOMO: -6.55794 LUMO: -0.27483 factor:1 | -1 (0.20158) | -1 | -1 |
| G: -6257.50192 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.77752 HOMO: -7.07496 LUMO: -0.63403 factor:1 | -1 (0.09010) | -1 | -1 |
| G: -6257.50192 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.85831 HOMO: -7.12394 LUMO: 0.53334 factor:1 | -1 (0.00931) | -1 | -1 |
| G: -6257.50192 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.91202 HOMO: -6.53617 LUMO: -0.25579 factor:1 | 1 (-0.04441) | -1 | -1 |
| G: -6257.50192 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.72941 HOMO: -6.50896 LUMO: -0.25034 factor:1 | -1 (0.13821) | -1 | -1 |
| G: -6257.50192 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.08182 HOMO: -7.17564 LUMO: -0.68573 factor:1 | 1 (-0.21421) | -1 | -1 |
| G: -6257.50192 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.89028 HOMO: -6.53617 LUMO: -0.30749 factor:1 | 1 (-0.02267) | -1 | -1 |
| G: -6257.50192 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.22928 HOMO: -6.55522 LUMO: -0.30749 factor:1 | 1 (-0.36167) | -1 | -1 |
| G: -6257.50192 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.52930 HOMO: -7.05591 LUMO: -0.71022 factor:1 | -1 (0.33832) | -1 | -1 |
| G: -6257.50192 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.82827 HOMO: -7.17564 LUMO: -0.69933 factor:1 | -1 (0.03935) | -1 | -1 |
| G: -6257.50192 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.12403 HOMO: -6.78380 LUMO: -0.67756 factor:1 | 1 (-0.25641) | -1 | -1 |
| G: -6257.50192 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.61003 HOMO: -6.62325 LUMO: 2.02725 factor:1 | -1 (0.25758) | 1 | 1 |
| G: -6257.50192 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.58375 HOMO: -6.63414 LUMO: 1.91296 factor:1 | -1 (0.28387) | 1 | -1 |
| G: -6257.50192 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.12642 HOMO: -6.83278 LUMO: 1.65717 factor:1 | 1 (-0.25881) | 1 | 1 |
| G: -6257.50192 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.35562 HOMO: -6.66407 LUMO: 1.95650 factor:1 | 1 (-0.48801) | 1 | 1 |
| G: -6257.50192 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.23274 HOMO: -6.61237 LUMO: 2.11432 factor:1 | 1 (-0.36512) | 1 | 1 |
| G: -6257.50192 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.21165 HOMO: -6.62053 LUMO: 2.09256 factor:1 | 1 (-0.34403) | 1 | -1 |
| G: -6257.50192 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.88163 HOMO: -6.78652 LUMO: 2.13609 factor:1 | 1 (-0.01401) | 1 | 1 |
| G: -6257.50192 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.00672 HOMO: -6.94707 LUMO: 1.81772 factor:1 | 1 (-0.13910) | 1 | 1 |
| G: -6257.50192 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.79153 HOMO: -6.85183 LUMO: 2.12793 factor:1 | -1 (0.07608) | 1 | 1 |
| G: -6257.50192 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.84508 HOMO: -6.81101 LUMO: 1.83949 factor:1 | -1 (0.02253) | 1 | 1 |
| G: -6257.50192 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.09393 HOMO: -6.98788 LUMO: 2.16058 factor:1 | 1 (-0.22632) | 1 | 1 |
| G: -6257.50192 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.19750 HOMO: -6.62869 LUMO: 2.00820 factor:1 | 1 (-0.32988) | 1 | 1 |
| G: -6257.50192 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.58807 HOMO: -6.34025 LUMO: 2.25855 factor:1 | -1 (0.27954) | -1 | -1 |
| G: -6257.50192 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.09336 HOMO: -6.01372 LUMO: 2.01636 factor:1 | 1 (-0.22575) | -1 | -1 |
| G: -6257.50192 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.68761 HOMO: -6.89264 LUMO: 2.27487 factor:1 | -1 (0.18000) | 1 | 1 |
| G: -6257.50192 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.79880 HOMO: -6.53073 LUMO: 2.20684 factor:1 | -1 (0.06882) | -1 | -1 |
| G: -6257.50192 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.79542 HOMO: -6.83278 LUMO: 1.53744 factor:1 | -1 (0.07219) | -1 | -1 |
| G: -6257.50192 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.73110 HOMO: -6.41917 LUMO: 1.82316 factor:1 | -1 (0.13652) | -1 | -1 |
| G: -6257.50192 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.05137 HOMO: -6.56339 LUMO: 1.63813 factor:1 | 1 (-0.18376) | -1 | -1 |
| G: -6257.50192 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.47876 HOMO: -6.88992 LUMO: 1.65173 factor:1 | 1 (-0.61114) | 1 | 1 |
| G: -6257.50192 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.69294 HOMO: -6.63141 LUMO: 1.92112 factor:1 | 1 (-0.82532) | 1 | 1 |
| G: -6257.50192 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.84535 HOMO: -6.83822 LUMO: 1.88847 factor:1 | 1 (-0.97773) | 1 | 1 |
| G: -6257.50192 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.58589 HOMO: -6.84638 LUMO: 1.90480 factor:1 | 1 (-0.71827) | 1 | 1 |
| G: -6257.50192 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.60540 HOMO: -6.82462 LUMO: 1.70888 factor:1 | 1 (-0.73778) | 1 | 1 |
| G: -6257.50192 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.62266 HOMO: -6.82734 LUMO: 2.12521 factor:1 | -1 (0.24496) | 1 | 1 |
| G: -6257.50192 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.63870 HOMO: -6.94435 LUMO: 1.87214 factor:1 | 1 (-0.77109) | 1 | 1 |
| G: -6257.50192 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.59772 HOMO: -6.98516 LUMO: 2.51433 factor:1 | 1 (-0.73011) | 1 | 1 |
| G: -6257.50192 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.55383 HOMO: -6.74026 LUMO: 2.15514 factor:1 | 1 (-0.68622) | 1 | 1 |
| G: -6257.50192 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.79552 HOMO: -6.93618 LUMO: 2.54426 factor:1 | 1 (-0.92791) | 1 | 1 |
| G: -6257.50192 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.40649 HOMO: -6.28583 LUMO: 2.53610 factor:1 | -1 (0.46112) | -1 | -1 |
| G: -6257.50192 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.47501 HOMO: -6.56883 LUMO: 1.94834 factor:1 | -1 (0.39261) | 1 | 1 |
| G: -6257.50192 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.98737 HOMO: -7.08584 LUMO: 1.99187 factor:1 | 1 (-0.11976) | 1 | 1 |
| G: -6257.50192 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.86498 HOMO: -6.19059 LUMO: 1.99732 factor:1 | -1 (0.00264) | -1 | -1 |
| G: -6257.50192 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.94389 HOMO: -6.78108 LUMO: 2.03813 factor:1 | 1 (-0.07627) | 1 | 1 |
| G: -6257.50192 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.62715 HOMO: -6.82189 LUMO: 1.77418 factor:1 | -1 (0.24047) | 1 | 1 |
| G: -6257.50192 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.85216 HOMO: -6.45454 LUMO: 1.78779 factor:1 | -1 (0.01546) | -1 | -1 |
| G: -6257.50192 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.83869 HOMO: -6.84366 LUMO: 1.77690 factor:1 | -1 (0.02893) | 1 | 1 |
| G: -6257.50192 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.93611 HOMO: -6.74026 LUMO: 1.67622 factor:1 | 1 (-0.06849) | 1 | 1 |
| G: -6257.50192 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.62160 HOMO: -6.76475 LUMO: 2.40277 factor:1 | -1 (0.24602) | 1 | 1 |
| G: -6257.50192 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.04512 HOMO: -6.65863 LUMO: 1.86670 factor:1 | 1 (-0.17750) | 1 | 1 |
| G: -6257.50192 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.91153 HOMO: -6.50080 LUMO: 1.93201 factor:1 | 1 (-0.04392) | -1 | -1 |
| G: -6257.50192 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.96087 HOMO: -6.34842 LUMO: 1.70888 factor:1 | 1 (-0.09325) | -1 | -1 |
| G: -6257.50192 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.87172 HOMO: -6.60692 LUMO: 2.20140 factor:1 | 1 (-0.00411) | 1 | 1 |
| G: -6257.50192 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.92000 HOMO: -6.74026 LUMO: 2.14970 factor:1 | 1 (-0.05238) | 1 | 1 |
| G: -6257.50192 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.84560 HOMO: -6.63686 LUMO: 2.17419 factor:1 | -1 (0.02201) | 1 | 1 |
| G: -6257.50192 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.60364 HOMO: -6.81917 LUMO: 2.10072 factor:1 | -1 (0.26398) | 1 | -1 |
| G: -6257.50192 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.73325 HOMO: -6.92802 LUMO: 2.04358 factor:1 | -1 (0.13437) | 1 | 1 |
| G: -6257.50192 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.52173 HOMO: -6.56067 LUMO: -0.47620 factor:1 | -1 (0.34588) | -1 | -1 |
| G: -6257.50192 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.89953 HOMO: -6.56611 LUMO: -0.77008 factor:1 | 1 (-1.03191) | -1 | -1 |
| G: -6257.50192 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.63043 HOMO: -6.78380 LUMO: -0.64763 factor:1 | 1 (-0.76282) | -1 | -1 |
| G: -6257.50192 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.56167 HOMO: -6.51985 LUMO: -0.24490 factor:1 | 1 (-0.69405) | -1 | -1 |
| G: -6257.50192 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.48286 HOMO: -6.52529 LUMO: -0.27483 factor:1 | 1 (-1.61524) | -1 | -1 |
| G: -6257.50192 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12524.17120 HOMO: -7.10489 LUMO: -0.62586 factor:1 | 1 (-2.30358) | -1 | -1 |
| G: -6257.50192 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12524.30905 HOMO: -7.18108 LUMO: 0.48980 factor:1 | 1 (-2.44143) | -1 | -1 |
| G: -6257.50192 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.37243 HOMO: -7.14299 LUMO: -0.63947 factor:1 | 1 (-1.50482) | -1 | -1 |
| G: -6257.50192 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.32321 HOMO: -6.70761 LUMO: -0.54423 factor:1 | 1 (-1.45559) | -1 | -1 |
| G: -6257.50192 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.52593 HOMO: -7.32258 LUMO: -1.03675 factor:1 | 1 (-1.65832) | -1 | -1 |
| G: -6257.50192 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12524.09813 HOMO: -6.65046 LUMO: -0.41361 factor:1 | 1 (-2.23052) | -1 | -1 |
| G: -6257.50192 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.96129 HOMO: -6.76475 LUMO: -0.60137 factor:1 | 1 (-2.09367) | -1 | -1 |
| G: -6257.50192 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12524.13846 HOMO: -6.77836 LUMO: -0.54423 factor:1 | 1 (-2.27084) | -1 | -1 |
| G: -6257.50192 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.45589 HOMO: -7.52395 LUMO: 0.26395 factor:1 | 1 (-1.58827) | -1 | -1 |
| G: -6257.50192 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12524.12113 HOMO: -6.93890 LUMO: -0.72382 factor:1 | 1 (-2.25351) | -1 | -1 |
| G: -6257.50192 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12524.58731 HOMO: -6.72938 LUMO: -0.47348 factor:1 | 1 (-2.71970) | -1 | -1 |
| G: -6257.50192 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.46388 HOMO: -6.66951 LUMO: -0.40817 factor:1 | -1 (0.40374) | -1 | -1 |
| G: -6257.50192 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.45544 HOMO: -6.60420 LUMO: -0.19320 factor:1 | 1 (-0.58782) | -1 | -1 |
| G: -6257.50192 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.22528 HOMO: -6.67495 LUMO: -0.27211 factor:1 | 1 (-0.35767) | -1 | -1 |
| G: -6257.50192 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12524.17193 HOMO: -7.23823 LUMO: -0.62858 factor:1 | 1 (-2.30431) | -1 | -1 |
| G: -6257.50192 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.49543 HOMO: -7.27088 LUMO: 0.53334 factor:1 | 1 (-1.62781) | -1 | -1 |
| G: -6257.50192 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12524.37136 HOMO: -7.20013 LUMO: 0.59049 factor:1 | 1 (-2.50375) | -1 | -1 |
| G: -6257.50192 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.79645 HOMO: -6.60148 LUMO: -0.20953 factor:1 | 1 (-0.92883) | -1 | -1 |
| G: -6257.50192 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.40002 HOMO: -6.69400 LUMO: -0.51974 factor:1 | -1 (0.46760) | -1 | -1 |
| G: -6257.50192 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.52273 HOMO: -7.40422 LUMO: -0.98777 factor:1 | 1 (-0.65511) | -1 | -1 |
| G: -6257.50192 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.50248 HOMO: -6.88176 LUMO: -0.71022 factor:1 | 1 (-0.63487) | -1 | -1 |
| G: -6257.50192 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.40896 HOMO: -6.86271 LUMO: -0.59321 factor:1 | 1 (-0.54134) | -1 | -1 |
| G: -6257.50192 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.53791 HOMO: -6.73754 LUMO: -0.55239 factor:1 | 1 (-0.67030) | -1 | -1 |
| G: -6257.50192 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.92102 HOMO: -6.71033 LUMO: 1.57010 factor:1 | 1 (-1.05341) | -1 | -1 |
| G: -6257.50192 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.50765 HOMO: -6.69672 LUMO: 1.68711 factor:1 | 1 (-0.64004) | 1 | 1 |
| G: -6257.50192 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.31839 HOMO: -6.67495 LUMO: 2.03813 factor:1 | 1 (-1.45078) | 1 | 1 |
| G: -6257.50192 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.31583 HOMO: -6.54434 LUMO: 1.83677 factor:1 | 1 (-1.44822) | -1 | -1 |
| G: -6257.50192 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.52610 HOMO: -6.57155 LUMO: 1.77146 factor:1 | 1 (-1.65848) | 1 | 1 |
| G: -6257.50192 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.28930 HOMO: -6.76747 LUMO: 1.87759 factor:1 | 1 (-1.42169) | 1 | 1 |
| G: -6257.50192 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.65620 HOMO: -6.58243 LUMO: 1.61364 factor:1 | 1 (-0.78859) | 1 | 1 |
| G: -6257.50192 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.99082 HOMO: -6.61781 LUMO: 2.13881 factor:1 | 1 (-1.12320) | 1 | 1 |
| G: -6257.50192 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.12658 HOMO: -6.62597 LUMO: 2.00276 factor:1 | 1 (-1.25896) | 1 | 1 |
| G: -6257.50192 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.99175 HOMO: -7.01237 LUMO: 1.95922 factor:1 | 1 (-1.12413) | 1 | 1 |
| G: -6257.50192 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.44431 HOMO: -7.03959 LUMO: 2.16875 factor:1 | 1 (-0.57669) | 1 | 1 |
| G: -6257.50192 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.58355 HOMO: -6.83278 LUMO: 1.91296 factor:1 | 1 (-0.71593) | 1 | 1 |
| G: -6257.50192 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.67383 HOMO: -6.40012 LUMO: 1.95650 factor:1 | 1 (-0.80622) | -1 | -1 |
| G: -6257.50192 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.56475 HOMO: -6.50080 LUMO: 1.73337 factor:1 | -1 (0.30286) | -1 | -1 |
| G: -6257.50192 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.26932 HOMO: -6.95795 LUMO: 2.28848 factor:1 | -1 (0.59830) | 1 | 1 |
| G: -6257.50192 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.83972 HOMO: -6.63686 LUMO: 2.20140 factor:1 | 1 (-0.97210) | 1 | -1 |
| G: -6257.50192 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.26192 HOMO: -6.57427 LUMO: 1.87214 factor:1 | -1 (0.60570) | 1 | -1 |
| G: -6257.50192 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.95792 HOMO: -6.38379 LUMO: 2.32113 factor:1 | 1 (-1.09031) | -1 | -1 |
| G: -6257.50192 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.96358 HOMO: -6.63958 LUMO: 2.04902 factor:1 | 1 (-1.09597) | 1 | 1 |
| G: -6257.50192 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.29568 HOMO: -6.70216 LUMO: 1.93201 factor:1 | 1 (-0.42806) | 1 | 1 |
| G: -6257.50192 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.43312 HOMO: -6.80557 LUMO: 2.23678 factor:1 | 1 (-0.56551) | 1 | 1 |
| G: -6257.50192 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.17391 HOMO: -6.72938 LUMO: 2.28304 factor:1 | 1 (-0.30629) | 1 | 1 |
| G: -6257.50192 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.18406 HOMO: -6.56067 LUMO: 1.66806 factor:1 | 1 (-0.31644) | -1 | -1 |
| G: -6257.50192 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.13758 HOMO: -6.95523 LUMO: 2.33474 factor:1 | 1 (-0.26996) | 1 | 1 |
| G: -6257.50192 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.16479 HOMO: -6.59876 LUMO: 2.30480 factor:1 | 1 (-0.29718) | 1 | 1 |
| G: -6257.50192 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12524.13188 HOMO: -6.87360 LUMO: 1.75786 factor:1 | 1 (-2.26426) | 1 | 1 |
| G: -6257.50192 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12524.35163 HOMO: -7.06408 LUMO: 1.99187 factor:1 | 1 (-2.48402) | 1 | 1 |
| G: -6257.50192 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.95448 HOMO: -6.95795 LUMO: 1.88847 factor:1 | 1 (-2.08687) | 1 | 1 |
| G: -6257.50192 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.40231 HOMO: -6.85455 LUMO: 1.63813 factor:1 | 1 (-1.53469) | 1 | 1 |
| G: -6257.50192 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.90943 HOMO: -7.09129 LUMO: 2.31569 factor:1 | 1 (-1.04182) | 1 | 1 |
| G: -6257.50192 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.65658 HOMO: -6.91441 LUMO: 1.68983 factor:1 | 1 (-0.78897) | 1 | 1 |
| G: -6257.50192 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.46491 HOMO: -6.89809 LUMO: 2.23678 factor:1 | -1 (0.40270) | 1 | 1 |
| G: -6257.50192 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.48987 HOMO: -6.78652 LUMO: 1.98371 factor:1 | -1 (0.37775) | 1 | -1 |
| G: -6257.50192 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.50251 HOMO: -6.94707 LUMO: 2.23678 factor:1 | 1 (-0.63490) | 1 | 1 |
| G: -6257.50192 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.45789 HOMO: -7.07224 LUMO: 2.13337 factor:1 | 1 (-0.59027) | 1 | 1 |
| G: -6257.50192 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.37499 HOMO: -6.94979 LUMO: 2.28031 factor:1 | 1 (-1.50737) | 1 | 1 |
| G: -6257.50192 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.93501 HOMO: -6.60965 LUMO: 2.20412 factor:1 | 1 (-1.06739) | 1 | 1 |
| G: -6257.50192 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.98151 HOMO: -6.87360 LUMO: 2.40277 factor:1 | 1 (-1.11390) | 1 | -1 |
| G: -6257.50192 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.03251 HOMO: -6.92802 LUMO: 1.89663 factor:1 | 1 (-1.16489) | 1 | -1 |
| G: -6257.50192 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.88943 HOMO: -6.88448 LUMO: 2.02725 factor:1 | 1 (-1.02181) | 1 | 1 |
| G: -6257.50192 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.93950 HOMO: -6.69128 LUMO: 1.55105 factor:1 | 1 (-1.07188) | -1 | -1 |
| G: -6257.50192 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.35462 HOMO: -6.54978 LUMO: 1.93201 factor:1 | 1 (-0.48700) | -1 | -1 |
| G: -6257.50192 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.36714 HOMO: -6.19331 LUMO: 1.46941 factor:1 | 1 (-0.49952) | -1 | -1 |
| G: -6257.50192 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.87041 HOMO: -6.55794 LUMO: 1.89663 factor:1 | 1 (-1.00279) | -1 | -1 |
| G: -6257.50192 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.96310 HOMO: -6.07630 LUMO: 1.94289 factor:1 | 1 (-0.09548) | -1 | -1 |
| G: -6257.50192 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.79710 HOMO: -7.46408 LUMO: 0.31565 factor:1 | 1 (-0.92949) | -1 | -1 |
| G: -6257.50192 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.36649 HOMO: -6.63958 LUMO: -0.61770 factor:1 | -1 (0.50112) | -1 | -1 |
| G: -6257.50192 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.29909 HOMO: -6.81101 LUMO: -0.57960 factor:1 | -1 (0.56853) | -1 | -1 |
| G: -6257.50192 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.24926 HOMO: -6.74298 LUMO: -0.57960 factor:1 | -1 (0.61835) | -1 | -1 |
| G: -6257.50192 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.11386 HOMO: -6.63686 LUMO: -0.42994 factor:1 | -1 (0.75376) | -1 | -1 |
| G: -6257.50192 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.65636 HOMO: -6.60965 LUMO: -0.41089 factor:1 | 1 (-0.78875) | -1 | -1 |
| G: -6257.50192 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.11158 HOMO: -6.60692 LUMO: -0.80274 factor:1 | 1 (-1.24397) | -1 | -1 |
| G: -6257.50192 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.21375 HOMO: -6.58788 LUMO: -0.78097 factor:1 | -1 (0.65386) | -1 | -1 |
| G: -6257.50192 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.96359 HOMO: -6.67767 LUMO: -0.48436 factor:1 | 1 (-0.09597) | -1 | -1 |
| G: -6257.50192 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.71280 HOMO: -6.63141 LUMO: -0.40545 factor:1 | 1 (-0.84519) | -1 | -1 |
| G: -6257.50192 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.83849 HOMO: -6.62053 LUMO: -0.83811 factor:1 | 1 (-0.97088) | -1 | -1 |
| G: -6257.50192 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.92521 HOMO: -6.59604 LUMO: -0.35375 factor:1 | 1 (-1.05760) | -1 | -1 |
| G: -6257.50192 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.24126 HOMO: -6.34297 LUMO: -0.39729 factor:1 | 1 (-0.37364) | -1 | -1 |
| G: -6257.50192 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.60239 HOMO: -6.67223 LUMO: 1.97827 factor:1 | -1 (0.26523) | 1 | 1 |
| G: -6257.50192 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.29014 HOMO: -6.40012 LUMO: 1.89935 factor:1 | -1 (0.57748) | -1 | -1 |
| G: -6257.50192 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.68124 HOMO: -6.74842 LUMO: 1.97283 factor:1 | -1 (0.18637) | 1 | -1 |
| G: -6257.50192 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.44622 HOMO: -6.76747 LUMO: 2.17147 factor:1 | -1 (0.42140) | 1 | 1 |
| G: -6257.50192 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.48192 HOMO: -6.72121 LUMO: 1.55649 factor:1 | -1 (0.38569) | -1 | -1 |
| G: -6257.50192 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.11249 HOMO: -6.97700 LUMO: 2.04085 factor:1 | 1 (-0.24488) | 1 | 1 |
| G: -6257.50192 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.90008 HOMO: -7.06680 LUMO: 2.04085 factor:1 | 1 (-0.03246) | 1 | -1 |
| G: -6257.50192 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.39686 HOMO: -7.09673 LUMO: 2.35106 factor:1 | -1 (0.47076) | 1 | 1 |
| G: -6257.50192 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.99897 HOMO: -6.83006 LUMO: 2.14970 factor:1 | 1 (-0.13135) | 1 | 1 |
| G: -6257.50192 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.98465 HOMO: -6.72665 LUMO: 2.20140 factor:1 | 1 (-0.11704) | 1 | -1 |
| G: -6257.50192 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.89777 HOMO: -6.77291 LUMO: 2.34562 factor:1 | 1 (-0.03015) | 1 | -1 |
| G: -6257.50192 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.95110 HOMO: -6.73754 LUMO: 2.00276 factor:1 | 1 (-0.08348) | 1 | -1 |
| G: -6257.50192 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.98846 HOMO: -7.04231 LUMO: 1.92112 factor:1 | 1 (-0.12085) | 1 | -1 |
| G: -6257.50192 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.95695 HOMO: -6.83822 LUMO: 1.72248 factor:1 | 1 (-0.08933) | 1 | 1 |
| G: -6257.50192 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.72609 HOMO: -6.57971 LUMO: 2.16603 factor:1 | -1 (0.14153) | 1 | -1 |
| G: -6257.50192 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.83183 HOMO: -6.80013 LUMO: 1.88575 factor:1 | -1 (0.03578) | 1 | 1 |
| G: -6257.50192 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.33337 HOMO: -6.93618 LUMO: 2.18235 factor:1 | 1 (-0.46575) | 1 | 1 |
| G: -6257.50192 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.19328 HOMO: -6.54706 LUMO: 1.91024 factor:1 | 1 (-0.32567) | -1 | -1 |
| G: -6257.50192 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.40663 HOMO: -7.06952 LUMO: 2.18507 factor:1 | -1 (0.46099) | 1 | 1 |
| G: -6257.50192 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.15860 HOMO: -7.05047 LUMO: 1.82044 factor:1 | -1 (0.70902) | 1 | 1 |
| G: -6257.50192 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.21857 HOMO: -6.87632 LUMO: 1.92657 factor:1 | -1 (0.64905) | 1 | 1 |
| G: -6257.50192 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.20834 HOMO: -6.58788 LUMO: 1.91568 factor:1 | -1 (0.65928) | 1 | -1 |
| G: -6257.50192 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.17754 HOMO: -7.17292 LUMO: 1.90752 factor:1 | -1 (0.69008) | 1 | 1 |
| G: -6257.50192 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.08834 HOMO: -6.93890 LUMO: 1.80684 factor:1 | -1 (0.77928) | 1 | 1 |
| G: -6257.50192 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.32369 HOMO: -7.10761 LUMO: 2.20956 factor:1 | -1 (0.54393) | 1 | 1 |
| G: -6257.50192 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.16401 HOMO: -6.85727 LUMO: 2.13609 factor:1 | -1 (0.70360) | 1 | -1 |
| G: -6257.50192 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.89379 HOMO: -6.64502 LUMO: 1.38506 factor:1 | 1 (-0.02618) | -1 | -1 |
| G: -6257.50192 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.99709 HOMO: -6.87360 LUMO: 1.15648 factor:1 | 1 (-0.12947) | -1 | -1 |
| G: -6257.50192 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.85186 HOMO: -6.67223 LUMO: 2.07351 factor:1 | -1 (0.01576) | 1 | 1 |
| G: -6257.50192 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.95094 HOMO: -6.29671 LUMO: 2.43270 factor:1 | 1 (-0.08332) | -1 | -1 |
| G: -6257.50192 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12520.83870 HOMO: -6.90897 LUMO: 2.28848 factor:1 | -1 (1.02892) | 1 | 1 |
| G: -6257.50192 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12520.83818 HOMO: -7.04231 LUMO: 1.70071 factor:1 | -1 (1.02943) | 1 | 1 |
| G: -6257.50192 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.22006 HOMO: -6.69944 LUMO: 1.94834 factor:1 | 1 (-0.35244) | 1 | 1 |
| G: -6257.50192 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.10108 HOMO: -6.56067 LUMO: 2.20956 factor:1 | 1 (-1.23346) | -1 | -1 |
| G: -6257.50192 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.21779 HOMO: -6.65046 LUMO: 2.06807 factor:1 | 1 (-1.35017) | 1 | -1 |
| G: -6257.50192 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12520.84180 HOMO: -7.08584 LUMO: 1.98915 factor:1 | -1 (1.02581) | 1 | 1 |
| G: -6257.50192 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.77397 HOMO: -6.69400 LUMO: 2.09256 factor:1 | 1 (-0.90636) | 1 | 1 |
| G: -6257.50192 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.91170 HOMO: -6.62869 LUMO: 2.16331 factor:1 | 1 (-0.04408) | 1 | 1 |
| G: -6257.50192 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.62646 HOMO: -6.85183 LUMO: 2.16058 factor:1 | 1 (-0.75884) | 1 | 1 |
| G: -6257.50192 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.83118 HOMO: -6.54706 LUMO: 1.92384 factor:1 | -1 (0.03644) | -1 | -1 |
| G: -6257.50192 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.87894 HOMO: -6.84366 LUMO: 2.48984 factor:1 | 1 (-0.01132) | 1 | 1 |
| G: -6257.50192 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.64260 HOMO: -6.77291 LUMO: 2.46263 factor:1 | -1 (0.22501) | 1 | 1 |
| G: -6257.50192 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.53651 HOMO: -7.01782 LUMO: 2.31025 factor:1 | -1 (0.33111) | 1 | 1 |
| G: -6257.50192 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.48418 HOMO: -6.94707 LUMO: 2.29664 factor:1 | -1 (0.38344) | 1 | 1 |
| G: -6257.50192 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.57117 HOMO: -6.64230 LUMO: 1.97283 factor:1 | -1 (0.29644) | 1 | 1 |
| G: -6257.50192 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.17500 HOMO: -6.47359 LUMO: 2.20412 factor:1 | 1 (-0.30738) | -1 | -1 |
| G: -6257.50192 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.24885 HOMO: -6.90625 LUMO: 1.92384 factor:1 | 1 (-0.38123) | 1 | 1 |
| G: -6257.50192 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.57353 HOMO: -7.17020 LUMO: 2.06807 factor:1 | 1 (-0.70592) | 1 | 1 |
| G: -6257.50192 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.25187 HOMO: -6.65046 LUMO: 2.20956 factor:1 | 1 (-0.38425) | 1 | -1 |
| G: -6257.50192 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.74263 HOMO: -7.07496 LUMO: 1.82861 factor:1 | -1 (0.12498) | 1 | 1 |
| G: -6257.50192 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.59893 HOMO: -6.83006 LUMO: 2.14970 factor:1 | -1 (0.26869) | 1 | -1 |
| G: -6257.50192 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.59275 HOMO: -6.92802 LUMO: 1.99187 factor:1 | -1 (0.27486) | 1 | 1 |
| G: -6257.50192 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.90056 HOMO: -6.69672 LUMO: 2.36739 factor:1 | 1 (-1.03294) | 1 | -1 |
| G: -6257.50192 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.85259 HOMO: -7.13755 LUMO: 2.00276 factor:1 | 1 (-0.98497) | 1 | 1 |
| G: -6257.50192 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.50121 HOMO: -6.92530 LUMO: 2.25582 factor:1 | 1 (-0.63359) | 1 | 1 |
| G: -6257.50192 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.20487 HOMO: -6.77564 LUMO: 1.97827 factor:1 | 1 (-0.33726) | 1 | 1 |
| G: -6257.50192 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.09989 HOMO: -6.87904 LUMO: 1.60003 factor:1 | 1 (-0.23228) | 1 | 1 |
| G: -6257.50192 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.18321 HOMO: -6.62869 LUMO: 1.90480 factor:1 | 1 (-0.31560) | 1 | 1 |
| G: -6257.50192 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.12264 HOMO: -6.71033 LUMO: 1.54833 factor:1 | 1 (-0.25503) | -1 | -1 |
| G: -6257.50192 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.46306 HOMO: -6.74298 LUMO: 1.47486 factor:1 | -1 (0.40455) | -1 | -1 |
| G: -6257.50192 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.21772 HOMO: -6.77019 LUMO: 1.90480 factor:1 | 1 (-0.35010) | 1 | 1 |
| G: -6257.50192 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.44508 HOMO: -6.70489 LUMO: 1.99459 factor:1 | -1 (0.42254) | 1 | 1 |
| G: -6257.50192 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.66658 HOMO: -6.73482 LUMO: 2.08711 factor:1 | -1 (0.20104) | 1 | 1 |
| G: -6257.50192 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.34899 HOMO: -6.46543 LUMO: 1.73881 factor:1 | -1 (0.51862) | -1 | -1 |
| G: -6257.50192 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.51131 HOMO: -6.96067 LUMO: 2.26127 factor:1 | -1 (0.35631) | 1 | 1 |
| G: -6257.50192 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.50960 HOMO: -6.67767 LUMO: 2.10616 factor:1 | -1 (0.35802) | 1 | 1 |
| G: -6257.50192 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.29759 HOMO: -6.28855 LUMO: 2.35923 factor:1 | -1 (0.57002) | -1 | -1 |
| G: -6257.50192 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.31865 HOMO: -6.80285 LUMO: 1.62724 factor:1 | -1 (0.54896) | 1 | 1 |
| G: -6257.50192 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.58481 HOMO: -6.85455 LUMO: 2.23133 factor:1 | -1 (0.28281) | 1 | 1 |
| G: -6257.50192 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.00476 HOMO: -6.51713 LUMO: 2.33474 factor:1 | 1 (-0.13715) | -1 | -1 |
| G: -6257.50192 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.14425 HOMO: -6.88176 LUMO: 2.15242 factor:1 | 1 (-0.27663) | 1 | 1 |
| G: -6257.50192 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.04049 HOMO: -6.54434 LUMO: 2.32113 factor:1 | 1 (-0.17287) | -1 | -1 |
| G: -6257.50192 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.48168 HOMO: -6.62597 LUMO: 2.24222 factor:1 | -1 (0.38594) | 1 | 1 |
| G: -6257.50192 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.60941 HOMO: -6.74570 LUMO: 2.19868 factor:1 | -1 (0.25821) | 1 | 1 |
| G: -6257.50192 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.64856 HOMO: -6.62869 LUMO: 1.98915 factor:1 | 1 (-0.78094) | 1 | 1 |
| G: -6257.50192 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.65577 HOMO: -6.64502 LUMO: 2.13881 factor:1 | 1 (-0.78815) | 1 | 1 |
| G: -6257.50192 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.41448 HOMO: -6.95795 LUMO: 1.82316 factor:1 | 1 (-0.54687) | 1 | 1 |
| G: -6257.50192 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.97910 HOMO: -6.77291 LUMO: 1.36329 factor:1 | 1 (-0.11149) | -1 | -1 |
| G: -6257.50192 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.59928 HOMO: -6.45726 LUMO: 1.73064 factor:1 | -1 (0.26833) | -1 | -1 |
| G: -6257.50192 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.75019 HOMO: -6.49264 LUMO: 1.77418 factor:1 | 1 (-0.88257) | -1 | -1 |
| G: -6257.50192 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.72516 HOMO: -6.60420 LUMO: 2.20956 factor:1 | 1 (-0.85754) | 1 | 1 |
| G: -6257.50192 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.69296 HOMO: -6.56067 LUMO: 2.05718 factor:1 | 1 (-0.82535) | -1 | -1 |
| G: -6257.50192 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.53726 HOMO: -6.62597 LUMO: 1.70343 factor:1 | 1 (-0.66964) | 1 | 1 |
| G: -6257.50192 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.84064 HOMO: -6.69400 LUMO: 2.16875 factor:1 | 1 (-0.97302) | 1 | 1 |
| G: -6257.50192 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.65900 HOMO: -6.63958 LUMO: 2.11977 factor:1 | 1 (-0.79139) | 1 | 1 |
| G: -6257.50192 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.80399 HOMO: -6.92802 LUMO: 1.82044 factor:1 | 1 (-0.93637) | 1 | -1 |
| G: -6257.50192 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.59370 HOMO: -6.56339 LUMO: 2.30480 factor:1 | 1 (-0.72608) | -1 | -1 |
| G: -6257.50192 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.96656 HOMO: -6.63958 LUMO: 1.91024 factor:1 | 1 (-0.09894) | 1 | -1 |
| G: -6257.50192 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.13181 HOMO: -6.93074 LUMO: 2.05446 factor:1 | 1 (-0.26420) | 1 | 1 |
| G: -6257.50192 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.28335 HOMO: -6.61509 LUMO: 2.03813 factor:1 | 1 (-0.41574) | 1 | 1 |
| G: -6257.50192 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.14686 HOMO: -6.61237 LUMO: 1.91296 factor:1 | 1 (-0.27924) | 1 | -1 |
| G: -6257.50192 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.45818 HOMO: -6.86815 LUMO: 1.95378 factor:1 | 1 (-0.59057) | 1 | 1 |
| G: -6257.50192 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.12920 HOMO: -6.63686 LUMO: 1.70888 factor:1 | 1 (-0.26158) | 1 | 1 |
| G: -6257.50192 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.93759 HOMO: -6.57971 LUMO: 2.20140 factor:1 | 1 (-1.06998) | 1 | -1 |
| G: -6257.50192 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.84323 HOMO: -6.41100 LUMO: 1.96738 factor:1 | 1 (-0.97561) | -1 | -1 |
| G: -6257.50192 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.84344 HOMO: -6.90081 LUMO: 1.65989 factor:1 | 1 (-0.97583) | 1 | 1 |
| G: -6257.50192 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.72733 HOMO: -6.68312 LUMO: 1.97827 factor:1 | 1 (-0.85972) | 1 | -1 |
| G: -6257.50192 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.71226 HOMO: -6.65318 LUMO: 2.10888 factor:1 | 1 (-0.84464) | 1 | -1 |
| G: -6257.50192 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.48923 HOMO: -6.62053 LUMO: 2.28848 factor:1 | 1 (-0.62162) | 1 | -1 |
| G: -6257.50192 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.66213 HOMO: -6.65863 LUMO: 2.29664 factor:1 | 1 (-0.79452) | 1 | -1 |
| G: -6257.50192 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.39693 HOMO: -6.63958 LUMO: 2.07623 factor:1 | 1 (-0.52932) | 1 | -1 |
| G: -6257.50192 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.48186 HOMO: -6.58243 LUMO: 2.20684 factor:1 | 1 (-0.61424) | 1 | 1 |
| G: -6257.50192 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.65272 HOMO: -6.59332 LUMO: 2.05174 factor:1 | 1 (-0.78510) | 1 | -1 |
| G: -6257.50192 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.65824 HOMO: -6.95251 LUMO: 2.20140 factor:1 | 1 (-0.79063) | 1 | 1 |
| G: -6257.50192 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.58798 HOMO: -6.84638 LUMO: 2.39732 factor:1 | 1 (-0.72037) | 1 | 1 |
| G: -6257.50192 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.77601 HOMO: -6.86815 LUMO: 2.47896 factor:1 | 1 (-0.90840) | 1 | 1 |
| G: -6257.50192 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.73014 HOMO: -7.00693 LUMO: 2.43270 factor:1 | 1 (-0.86252) | 1 | 1 |
| G: -6257.50192 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.33897 HOMO: -6.58788 LUMO: 2.30208 factor:1 | 1 (-0.47136) | 1 | 1 |
| G: -6257.50192 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.08716 HOMO: -6.63958 LUMO: 2.28031 factor:1 | 1 (-0.21954) | 1 | 1 |
| G: -6257.50192 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.28224 HOMO: -6.74570 LUMO: 2.28304 factor:1 | 1 (-0.41462) | 1 | 1 |
| G: -6257.50192 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.30694 HOMO: -6.78380 LUMO: 2.16331 factor:1 | 1 (-0.43933) | 1 | 1 |
| G: -6257.50192 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.21391 HOMO: -6.52529 LUMO: 2.05718 factor:1 | 1 (-0.34629) | -1 | -1 |
| G: -6257.50192 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.16177 HOMO: -6.41644 LUMO: 1.65445 factor:1 | 1 (-0.29416) | -1 | -1 |
| G: -6257.50192 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.17600 HOMO: -6.34570 LUMO: 1.22451 factor:1 | 1 (-0.30839) | -1 | -1 |
| G: -6257.50192 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.18885 HOMO: -6.14433 LUMO: 1.85582 factor:1 | 1 (-0.32123) | -1 | -1 |
| G: -6257.50192 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.89114 HOMO: -6.62053 LUMO: 1.92112 factor:1 | 1 (-1.02353) | 1 | -1 |
| G: -6257.50192 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.86004 HOMO: -6.63414 LUMO: 1.61908 factor:1 | 1 (-0.99243) | 1 | 1 |
| G: -6257.50192 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.07295 HOMO: -6.75931 LUMO: 1.87214 factor:1 | 1 (-0.20534) | 1 | 1 |
| G: -6257.50192 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.15358 HOMO: -6.55794 LUMO: 1.77418 factor:1 | 1 (-0.28596) | -1 | -1 |
| G: -6257.50192 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.65412 HOMO: -6.52801 LUMO: 1.82044 factor:1 | -1 (0.21350) | -1 | -1 |
| G: -6257.50192 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.10887 HOMO: -6.77564 LUMO: 1.97827 factor:1 | 1 (-0.24126) | 1 | 1 |
| G: -6257.50192 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.75476 HOMO: -6.93890 LUMO: 1.81228 factor:1 | 1 (-0.88715) | 1 | 1 |
| G: -6257.50192 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.28955 HOMO: -6.85455 LUMO: 1.75513 factor:1 | 1 (-1.42193) | 1 | 1 |
| G: -6257.50192 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.77078 HOMO: -6.86815 LUMO: 1.64629 factor:1 | 1 (-1.90316) | 1 | 1 |
| G: -6257.50192 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.77043 HOMO: -6.98516 LUMO: 1.84765 factor:1 | 1 (-1.90281) | 1 | 1 |
| G: -6257.50192 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.87111 HOMO: -6.04637 LUMO: 1.94017 factor:1 | 1 (-2.00349) | -1 | -1 |
| G: -6257.50192 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.29801 HOMO: -6.86271 LUMO: 2.11977 factor:1 | 1 (-1.43039) | 1 | -1 |
| G: -6257.50192 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.50041 HOMO: -6.72938 LUMO: 2.11160 factor:1 | 1 (-1.63279) | 1 | -1 |
| G: -6257.50192 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.91244 HOMO: -7.01782 LUMO: 2.13609 factor:1 | 1 (-2.04483) | 1 | 1 |
| G: -6257.50192 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.50199 HOMO: -6.18515 LUMO: 2.04630 factor:1 | 1 (-1.63437) | -1 | -1 |
| G: -6257.50192 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12524.04134 HOMO: -6.60965 LUMO: 2.17147 factor:1 | 1 (-2.17373) | 1 | -1 |
| G: -6257.50192 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.30005 HOMO: -6.87360 LUMO: 2.35378 factor:1 | 1 (-1.43243) | 1 | 1 |
| G: -6257.50192 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.79747 HOMO: -6.72938 LUMO: 2.20140 factor:1 | 1 (-1.92986) | 1 | -1 |
| G: -6257.50192 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.84050 HOMO: -6.88448 LUMO: 2.54154 factor:1 | 1 (-1.97288) | 1 | -1 |
| G: -6257.50192 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12524.12725 HOMO: -6.87087 LUMO: 2.16058 factor:1 | 1 (-2.25963) | 1 | 1 |
| G: -6257.50192 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.90270 HOMO: -7.11306 LUMO: 2.04085 factor:1 | 1 (-2.03509) | 1 | 1 |
| G: -6257.50192 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.23512 HOMO: -6.66951 LUMO: 1.68438 factor:1 | 1 (-1.36751) | 1 | 1 |
| G: -6257.50192 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.72558 HOMO: -7.08312 LUMO: 2.19324 factor:1 | 1 (-1.85797) | 1 | 1 |
| G: -6257.50192 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.48778 HOMO: -6.69128 LUMO: 2.13881 factor:1 | 1 (-1.62017) | 1 | -1 |
| G: -6257.50192 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.29659 HOMO: -6.80285 LUMO: 2.16603 factor:1 | 1 (-1.42898) | 1 | 1 |
| G: -6257.50192 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.42117 HOMO: -6.82189 LUMO: 2.46807 factor:1 | 1 (-1.55355) | 1 | 1 |
| G: -6257.50192 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.30571 HOMO: -6.78652 LUMO: 2.12521 factor:1 | 1 (-1.43809) | 1 | 1 |
| G: -6257.50192 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.96056 HOMO: -6.47903 LUMO: 1.70071 factor:1 | 1 (-1.09295) | -1 | -1 |
| G: -6257.50192 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.10065 HOMO: -6.37019 LUMO: 1.24356 factor:1 | 1 (-1.23303) | -1 | -1 |
| G: -6257.50192 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.11431 HOMO: -6.69400 LUMO: 1.67350 factor:1 | 1 (-1.24669) | 1 | 1 |
| G: -6257.50192 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.15066 HOMO: -7.51851 LUMO: 0.27756 factor:1 | 1 (-1.28304) | -1 | -1 |
| G: -6257.50192 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.20723 HOMO: -6.95795 LUMO: -0.72110 factor:1 | 1 (-1.33962) | -1 | -1 |
| G: -6257.50192 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.23654 HOMO: -6.88720 LUMO: -0.67484 factor:1 | 1 (-1.36892) | -1 | -1 |
| G: -6257.50192 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12524.00091 HOMO: -6.83550 LUMO: -0.57144 factor:1 | 1 (-2.13329) | -1 | -1 |
| G: -6257.50192 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.73165 HOMO: -6.80285 LUMO: -0.57144 factor:1 | 1 (-1.86403) | -1 | -1 |
| G: -6257.50192 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.96580 HOMO: -6.76475 LUMO: -0.53062 factor:1 | 1 (-2.09819) | -1 | -1 |
| G: -6257.50192 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.25042 HOMO: -6.66951 LUMO: 1.74969 factor:1 | 1 (-1.38280) | 1 | 1 |
| G: -6257.50192 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.34876 HOMO: -6.53345 LUMO: 1.89935 factor:1 | 1 (-1.48114) | -1 | -1 |
| G: -6257.50192 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.92528 HOMO: -6.65046 LUMO: 2.01364 factor:1 | 1 (-0.05766) | 1 | -1 |
| G: -6257.50192 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.04046 HOMO: -6.64230 LUMO: 2.11977 factor:1 | 1 (-0.17285) | 1 | -1 |
| G: -6257.50192 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.79136 HOMO: -6.44910 LUMO: 2.13337 factor:1 | 1 (-0.92374) | -1 | -1 |
| G: -6257.50192 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.87267 HOMO: -7.05591 LUMO: 1.98915 factor:1 | 1 (-1.00505) | 1 | -1 |
| G: -6257.50192 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.15334 HOMO: -7.02326 LUMO: 2.49256 factor:1 | 1 (-0.28572) | 1 | 1 |
| G: -6257.50192 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.30003 HOMO: -6.32937 LUMO: 2.51161 factor:1 | 1 (-0.43242) | -1 | -1 |
| G: -6257.50192 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.25678 HOMO: -6.96067 LUMO: 2.20140 factor:1 | 1 (-1.38917) | 1 | 1 |
| G: -6257.50192 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.21970 HOMO: -6.97972 LUMO: 2.55243 factor:1 | 1 (-1.35208) | 1 | 1 |
| G: -6257.50192 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.29034 HOMO: -6.72665 LUMO: 2.46535 factor:1 | 1 (-1.42272) | 1 | 1 |
| G: -6257.50192 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.92988 HOMO: -6.41917 LUMO: 2.35106 factor:1 | 1 (-0.06226) | -1 | -1 |
| G: -6257.50192 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.06490 HOMO: -6.75114 LUMO: 2.32929 factor:1 | 1 (-0.19728) | 1 | 1 |
| G: -6257.50192 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.86846 HOMO: -6.91713 LUMO: 2.27215 factor:1 | 1 (-0.00084) | 1 | 1 |
| G: -6257.50192 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.83781 HOMO: -6.54978 LUMO: 2.00276 factor:1 | 1 (-0.97019) | -1 | -1 |
| G: -6257.50192 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.76807 HOMO: -6.62325 LUMO: 2.05990 factor:1 | 1 (-0.90045) | 1 | 1 |
| G: -6257.50192 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.90227 HOMO: -6.86271 LUMO: 2.14970 factor:1 | 1 (-1.03466) | 1 | 1 |
| G: -6257.50192 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.02304 HOMO: -6.77564 LUMO: 2.25855 factor:1 | 1 (-1.15542) | 1 | -1 |
| G: -6257.50192 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.79120 HOMO: -6.71305 LUMO: 1.94561 factor:1 | 1 (-0.92358) | 1 | -1 |
| G: -6257.50192 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.83381 HOMO: -6.75659 LUMO: 1.94561 factor:1 | 1 (-0.96619) | 1 | -1 |
| G: -6257.50192 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.99351 HOMO: -6.94979 LUMO: 2.33474 factor:1 | 1 (-1.12590) | 1 | -1 |
| G: -6257.50192 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.92878 HOMO: -6.85727 LUMO: 2.50345 factor:1 | 1 (-1.06116) | 1 | -1 |
| G: -6257.50192 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.53137 HOMO: -6.87360 LUMO: 2.43270 factor:1 | 1 (-1.66376) | 1 | -1 |
| G: -6257.50192 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.86368 HOMO: -6.57427 LUMO: 2.46807 factor:1 | 1 (-1.99606) | 1 | -1 |
| G: -6257.50192 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.73358 HOMO: -7.16204 LUMO: 2.15242 factor:1 | 1 (-1.86597) | 1 | 1 |
| G: -6257.50192 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.06429 HOMO: -6.62869 LUMO: 2.11432 factor:1 | 1 (-1.19668) | 1 | -1 |
| G: -6257.50192 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.08701 HOMO: -7.05591 LUMO: 2.26671 factor:1 | 1 (-1.21940) | 1 | -1 |
| G: -6257.50192 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.58389 HOMO: -7.13483 LUMO: 1.47758 factor:1 | 1 (-1.71628) | -1 | -1 |
| G: -6257.50192 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.88110 HOMO: -6.72938 LUMO: 1.57282 factor:1 | 1 (-1.01349) | -1 | -1 |
| G: -6257.50192 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.73476 HOMO: -6.17426 LUMO: 1.81228 factor:1 | 1 (-0.86715) | -1 | -1 |
| G: -6257.50192 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.80453 HOMO: -6.65318 LUMO: 1.93473 factor:1 | 1 (-0.93692) | 1 | -1 |
| G: -6257.50192 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.60711 HOMO: -6.18515 LUMO: 2.01364 factor:1 | 1 (-0.73950) | -1 | -1 |
| G: -6257.50192 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.35204 HOMO: -7.05591 LUMO: 2.13337 factor:1 | -1 (0.51557) | 1 | 1 |
| G: -6257.50192 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.27784 HOMO: -6.90897 LUMO: 2.29664 factor:1 | -1 (0.58978) | 1 | -1 |
| G: -6257.50192 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.56007 HOMO: -7.11034 LUMO: 2.17147 factor:1 | -1 (0.30754) | 1 | 1 |
| G: -6257.50192 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.30390 HOMO: -6.82734 LUMO: 2.26671 factor:1 | 1 (-0.43628) | 1 | 1 |
| G: -6257.50192 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.99030 HOMO: -6.34842 LUMO: 2.34562 factor:1 | 1 (-1.12269) | -1 | -1 |
| G: -6257.50192 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.81920 HOMO: -6.62053 LUMO: 2.22861 factor:1 | 1 (-0.95158) | 1 | -1 |
| G: -6257.50192 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.45037 HOMO: -6.80557 LUMO: 2.07079 factor:1 | 1 (-0.58276) | 1 | -1 |
| G: -6257.50192 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.48303 HOMO: -6.60692 LUMO: 2.46263 factor:1 | 1 (-0.61541) | 1 | -1 |
| G: -6257.50192 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.45427 HOMO: -7.02054 LUMO: 2.08711 factor:1 | -1 (0.41334) | 1 | -1 |
| G: -6257.50192 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.45193 HOMO: -6.78652 LUMO: 2.02453 factor:1 | -1 (0.41568) | 1 | 1 |
| G: -6257.50192 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.58043 HOMO: -6.51168 LUMO: 2.06534 factor:1 | -1 (0.28719) | -1 | -1 |
| G: -6257.50192 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.03197 HOMO: -6.50080 LUMO: 2.01636 factor:1 | 1 (-0.16436) | -1 | -1 |
| G: -6257.50192 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.14082 HOMO: -6.54434 LUMO: 1.84493 factor:1 | 1 (-0.27320) | -1 | -1 |
| G: -6257.50192 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.98449 HOMO: -6.47087 LUMO: 1.76330 factor:1 | 1 (-0.11687) | -1 | -1 |
| G: -6257.50192 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.47262 HOMO: -6.78924 LUMO: 2.39460 factor:1 | -1 (0.39500) | 1 | 1 |
| G: -6257.50192 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.50034 HOMO: -6.59876 LUMO: 1.84493 factor:1 | -1 (0.36727) | 1 | 1 |
| G: -6257.50192 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.41215 HOMO: -6.41644 LUMO: 2.05174 factor:1 | -1 (0.45546) | -1 | -1 |
| G: -6257.50192 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.10246 HOMO: -6.52257 LUMO: 2.11160 factor:1 | -1 (0.76516) | -1 | -1 |
| G: -6257.50192 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.52395 HOMO: -6.90897 LUMO: 2.34018 factor:1 | 1 (-0.65634) | 1 | 1 |
| G: -6257.50192 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.33709 HOMO: -6.97428 LUMO: 1.86126 factor:1 | 1 (-1.46947) | 1 | 1 |
| G: -6257.50192 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.26326 HOMO: -7.13483 LUMO: 2.14698 factor:1 | 1 (-1.39564) | 1 | -1 |
| G: -6257.50192 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.17261 HOMO: -7.16748 LUMO: 2.31841 factor:1 | -1 (0.69501) | 1 | 1 |
| G: -6257.50192 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.65367 HOMO: -6.87087 LUMO: 2.38916 factor:1 | 1 (-0.78606) | 1 | -1 |
| G: -6257.50192 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.65830 HOMO: -6.93074 LUMO: 2.42181 factor:1 | 1 (-0.79068) | 1 | -1 |
| G: -6257.50192 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.97205 HOMO: -6.90081 LUMO: 2.00276 factor:1 | 1 (-0.10444) | 1 | -1 |
| G: -6257.50192 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.75718 HOMO: -6.99333 LUMO: 2.03541 factor:1 | 1 (-0.88957) | 1 | 1 |
| G: -6257.50192 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.07176 HOMO: -6.89264 LUMO: 1.57554 factor:1 | 1 (-0.20414) | -1 | -1 |
| G: -6257.50192 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.18104 HOMO: -6.48175 LUMO: 1.85854 factor:1 | 1 (-0.31342) | -1 | -1 |
| G: -6257.50192 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.16109 HOMO: -6.69400 LUMO: 1.62452 factor:1 | 1 (-0.29347) | 1 | 1 |
| G: -6257.50192 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.16476 HOMO: -6.50896 LUMO: 1.88303 factor:1 | 1 (-0.29715) | -1 | -1 |
| G: -6257.50192 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.26278 HOMO: -6.60420 LUMO: 2.05990 factor:1 | 1 (-0.39516) | 1 | 1 |
| G: -6257.50192 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.13875 HOMO: -7.14299 LUMO: 2.07351 factor:1 | 1 (-0.27113) | 1 | 1 |
| G: -6257.50192 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.04691 HOMO: -7.06408 LUMO: 1.81228 factor:1 | 1 (-0.17930) | 1 | 1 |
| G: -6257.50192 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.14016 HOMO: -6.67495 LUMO: 1.79595 factor:1 | 1 (-0.27255) | 1 | 1 |
| G: -6257.50192 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.12095 HOMO: -6.45182 LUMO: 2.15786 factor:1 | 1 (-0.25334) | -1 | -1 |
| G: -6257.50192 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.05502 HOMO: -6.93346 LUMO: 2.45719 factor:1 | 1 (-0.18740) | 1 | 1 |
| G: -6257.50192 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.26006 HOMO: -6.50080 LUMO: 2.08167 factor:1 | 1 (-0.39244) | -1 | -1 |
| G: -6257.50192 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.05350 HOMO: -6.83550 LUMO: -0.67484 factor:1 | 1 (-0.18588) | -1 | -1 |
| G: -6257.50192 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.08523 HOMO: -7.04231 LUMO: 0.54151 factor:1 | 1 (-0.21761) | -1 | -1 |
| G: -6257.50192 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.09777 HOMO: -6.79740 LUMO: 1.91296 factor:1 | 1 (-0.23015) | -1 | -1 |
| G: -6257.50192 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.94922 HOMO: -7.35796 LUMO: -1.04220 factor:1 | 1 (-0.08161) | -1 | -1 |
| G: -6257.50192 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.82302 HOMO: -6.62597 LUMO: -0.44082 factor:1 | -1 (0.04460) | -1 | -1 |
| G: -6257.50192 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.04746 HOMO: -6.45182 LUMO: -0.20409 factor:1 | 1 (-0.17984) | -1 | -1 |
| G: -6257.50192 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.82310 HOMO: -6.51168 LUMO: -0.23130 factor:1 | -1 (0.04452) | -1 | -1 |
| G: -6257.50192 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.14226 HOMO: -7.14027 LUMO: 0.49797 factor:1 | 1 (-0.27464) | -1 | -1 |
| G: -6257.50192 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.42232 HOMO: -7.55660 LUMO: 0.24762 factor:1 | 1 (-0.55470) | -1 | -1 |
| G: -6257.50192 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.99584 HOMO: -6.88992 LUMO: -0.64763 factor:1 | 1 (-0.12822) | -1 | -1 |
| G: -6257.50192 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.99858 HOMO: -6.72665 LUMO: -0.45987 factor:1 | 1 (-0.13097) | -1 | -1 |
| G: -6257.50192 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.69120 HOMO: -6.72121 LUMO: -0.58232 factor:1 | -1 (0.17641) | -1 | -1 |
| G: -6257.50192 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.04898 HOMO: -7.26816 LUMO: 0.32926 factor:1 | 1 (-0.18136) | -1 | -1 |
| G: -6257.50192 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.10950 HOMO: -6.57155 LUMO: -0.53606 factor:1 | 1 (-0.24188) | -1 | -1 |
| G: -6257.50192 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.25317 HOMO: -6.50896 LUMO: -0.43810 factor:1 | 1 (-0.38556) | -1 | -1 |
| G: -6257.50192 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.12248 HOMO: -6.73210 LUMO: -0.51430 factor:1 | 1 (-0.25486) | -1 | -1 |
| G: -6257.50192 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.68709 HOMO: -6.77019 LUMO: -0.62858 factor:1 | 1 (-0.81947) | -1 | -1 |
| G: -6257.50192 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.67615 HOMO: -6.82462 LUMO: -0.67484 factor:1 | 1 (-0.80853) | -1 | -1 |
| G: -6257.50192 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.95093 HOMO: -6.79740 LUMO: -0.55511 factor:1 | 1 (-1.08331) | -1 | -1 |
| G: -6257.50192 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.95422 HOMO: -6.79740 LUMO: -0.67756 factor:1 | 1 (-1.08661) | -1 | -1 |
| G: -6257.50192 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.80363 HOMO: -6.75114 LUMO: -0.55239 factor:1 | 1 (-0.93602) | -1 | -1 |
| G: -6257.50192 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.94010 HOMO: -6.49536 LUMO: -0.25307 factor:1 | 1 (-1.07248) | -1 | -1 |
| G: -6257.50192 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.53753 HOMO: -6.48992 LUMO: -0.25034 factor:1 | 1 (-0.66992) | -1 | -1 |
| G: -6257.50192 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.10596 HOMO: -6.52801 LUMO: -0.28028 factor:1 | 1 (-0.23834) | -1 | -1 |
| G: -6257.50192 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.01905 HOMO: -7.22462 LUMO: 0.52518 factor:1 | 1 (-0.15143) | -1 | -1 |
| G: -6257.50192 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.64907 HOMO: -6.59332 LUMO: -0.27211 factor:1 | 1 (-0.78146) | -1 | -1 |
| G: -6257.50192 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.71925 HOMO: -6.57427 LUMO: -0.16871 factor:1 | 1 (-0.85163) | -1 | -1 |
| G: -6257.50192 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.78200 HOMO: -6.71033 LUMO: 1.59187 factor:1 | 1 (-0.91438) | -1 | -1 |
| G: -6257.50192 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.50937 HOMO: -6.72121 LUMO: 2.00004 factor:1 | 1 (-0.64175) | -1 | -1 |
| G: -6257.50192 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.87297 HOMO: -6.61509 LUMO: 1.55921 factor:1 | 1 (-1.00535) | -1 | -1 |
| G: -6257.50192 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.72702 HOMO: -6.55250 LUMO: 1.73064 factor:1 | 1 (-1.85941) | -1 | -1 |
| G: -6257.50192 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.13624 HOMO: -6.66135 LUMO: 2.02181 factor:1 | 1 (-1.26862) | -1 | -1 |
| G: -6257.50192 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.75655 HOMO: -6.84911 LUMO: 1.98099 factor:1 | 1 (-1.88893) | -1 | -1 |
| G: -6257.50192 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.00075 HOMO: -6.66679 LUMO: 1.98371 factor:1 | 1 (-1.13314) | -1 | -1 |
| G: -6257.50192 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.17031 HOMO: -6.67495 LUMO: 2.04085 factor:1 | 1 (-1.30269) | -1 | -1 |
| G: -6257.50192 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.79415 HOMO: -6.89809 LUMO: 1.95106 factor:1 | 1 (-1.92654) | -1 | -1 |
| G: -6257.50192 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.39894 HOMO: -6.50352 LUMO: 1.88847 factor:1 | 1 (-1.53132) | -1 | -1 |
| G: -6257.50192 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.78569 HOMO: -6.93618 LUMO: 2.00004 factor:1 | 1 (-1.91808) | -1 | -1 |
| G: -6257.50192 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.48101 HOMO: -6.50896 LUMO: 1.73609 factor:1 | 1 (-1.61339) | -1 | -1 |
| G: -6257.50192 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.75611 HOMO: -6.69672 LUMO: 2.37283 factor:1 | 1 (-1.88850) | -1 | -1 |
| G: -6257.50192 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.58561 HOMO: -6.65591 LUMO: 2.20684 factor:1 | 1 (-1.71799) | -1 | -1 |
| G: -6257.50192 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.84445 HOMO: -6.23957 LUMO: 1.78507 factor:1 | 1 (-0.97683) | -1 | -1 |
| G: -6257.50192 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.35355 HOMO: -6.35114 LUMO: 1.92112 factor:1 | 1 (-1.48593) | -1 | -1 |
| G: -6257.50192 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.95860 HOMO: -6.53617 LUMO: 1.75241 factor:1 | 1 (-1.09099) | -1 | -1 |
| G: -6257.50192 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.99852 HOMO: -6.60420 LUMO: 1.78779 factor:1 | 1 (-1.13091) | -1 | -1 |
| G: -6257.50192 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.40917 HOMO: -7.40422 LUMO: -0.97145 factor:1 | 1 (-1.54155) | -1 | -1 |
| G: -6257.50192 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.53524 HOMO: -6.80013 LUMO: -0.69117 factor:1 | 1 (-1.66762) | -1 | -1 |
| G: -6257.50192 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.31306 HOMO: -6.68040 LUMO: -0.47076 factor:1 | 1 (-1.44544) | -1 | -1 |
| G: -6257.50192 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.30677 HOMO: -7.20285 LUMO: -0.66124 factor:1 | 1 (-1.43916) | -1 | -1 |
| G: -6257.50192 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.20693 HOMO: -6.82734 LUMO: -0.60137 factor:1 | 1 (-1.33932) | -1 | -1 |
| G: -6257.50192 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.60982 HOMO: -7.18653 LUMO: 0.59321 factor:1 | 1 (-1.74221) | -1 | -1 |
| G: -6257.50192 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.13178 HOMO: -7.29265 LUMO: 0.48164 factor:1 | 1 (-0.26417) | -1 | -1 |
| G: -6257.50192 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.89694 HOMO: -6.63414 LUMO: -0.25034 factor:1 | 1 (-1.02933) | -1 | -1 |
| G: -6257.50192 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.87207 HOMO: -7.20285 LUMO: 0.53879 factor:1 | 1 (-1.00445) | -1 | -1 |
| G: -6257.50192 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.70935 HOMO: -6.46815 LUMO: -0.21769 factor:1 | 1 (-0.84173) | -1 | -1 |
| G: -6257.50192 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.99006 HOMO: -6.57971 LUMO: -0.18776 factor:1 | 1 (-1.12244) | -1 | -1 |
| G: -6257.50192 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.94832 HOMO: -6.90897 LUMO: 1.91296 factor:1 | 1 (-1.08070) | -1 | -1 |
| G: -6257.50192 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.87928 HOMO: -6.67495 LUMO: 2.04358 factor:1 | 1 (-1.01166) | -1 | -1 |
| G: -6257.50192 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.75590 HOMO: -6.94162 LUMO: 1.73881 factor:1 | 1 (-0.88829) | -1 | -1 |
| G: -6257.50192 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.98467 HOMO: -6.73482 LUMO: 1.95922 factor:1 | 1 (-1.11705) | -1 | -1 |
| G: -6257.50192 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.88630 HOMO: -6.70489 LUMO: 2.04358 factor:1 | 1 (-1.01869) | -1 | -1 |
| G: -6257.50192 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.97060 HOMO: -7.04231 LUMO: 1.79323 factor:1 | 1 (-1.10299) | -1 | -1 |
| G: -6257.50192 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.97213 HOMO: -6.68584 LUMO: 1.60275 factor:1 | 1 (-1.10451) | -1 | -1 |
| G: -6257.50192 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.13069 HOMO: -6.40556 LUMO: 1.45581 factor:1 | 1 (-1.26307) | -1 | -1 |
| G: -6257.50192 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.94949 HOMO: -6.94979 LUMO: 2.16603 factor:1 | 1 (-0.08188) | -1 | -1 |
| G: -6257.50192 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.88732 HOMO: -6.84911 LUMO: 1.89935 factor:1 | 1 (-0.01970) | -1 | -1 |
| G: -6257.50192 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.90658 HOMO: -6.22052 LUMO: 1.57282 factor:1 | 1 (-0.03897) | -1 | -1 |
| G: -6257.50192 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.74620 HOMO: -6.51168 LUMO: 2.10072 factor:1 | -1 (0.12142) | -1 | -1 |
| G: -6257.50192 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.11738 HOMO: -7.03686 LUMO: 2.12249 factor:1 | 1 (-1.24976) | -1 | -1 |
| G: -6257.50192 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.19409 HOMO: -6.84094 LUMO: 1.63268 factor:1 | 1 (-1.32647) | -1 | -1 |
| G: -6257.50192 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.10486 HOMO: -6.75387 LUMO: 1.72248 factor:1 | 1 (-1.23725) | -1 | -1 |
| G: -6257.50192 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.85483 HOMO: -6.86271 LUMO: 1.68711 factor:1 | -1 (0.01279) | -1 | -1 |
| G: -6257.50192 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.91815 HOMO: -6.84094 LUMO: 2.02997 factor:1 | 1 (-0.05053) | -1 | -1 |
| G: -6257.50192 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.72906 HOMO: -6.80557 LUMO: 2.02725 factor:1 | -1 (0.13856) | -1 | -1 |
| G: -6257.50192 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.72800 HOMO: -6.38651 LUMO: 1.53472 factor:1 | 1 (-1.86039) | -1 | -1 |
| G: -6257.50192 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.38343 HOMO: -7.51306 LUMO: 0.28572 factor:1 | 1 (-1.51581) | -1 | -1 |
| G: -6257.50192 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.48264 HOMO: -6.97972 LUMO: -0.74287 factor:1 | 1 (-1.61502) | -1 | -1 |
| G: -6257.50192 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.89912 HOMO: -6.83822 LUMO: -0.65852 factor:1 | 1 (-1.03150) | -1 | -1 |
| G: -6257.50192 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.61325 HOMO: -6.71305 LUMO: -0.49525 factor:1 | 1 (-1.74564) | -1 | -1 |
| G: -6257.50192 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.87384 HOMO: -6.60692 LUMO: -0.22313 factor:1 | 1 (-1.00622) | -1 | -1 |
| G: -6257.50192 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.74733 HOMO: -7.20013 LUMO: 0.55239 factor:1 | 1 (-0.87972) | -1 | -1 |
| G: -6257.50192 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.09597 HOMO: -6.60420 LUMO: -0.28028 factor:1 | 1 (-0.22836) | -1 | -1 |
| G: -6257.50192 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.98612 HOMO: -6.69128 LUMO: -0.30477 factor:1 | 1 (-0.11851) | -1 | -1 |
| G: -6257.50192 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.95616 HOMO: -6.65591 LUMO: -0.25579 factor:1 | 1 (-0.08855) | -1 | -1 |
| G: -6257.50192 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.11720 HOMO: -6.69128 LUMO: 1.70888 factor:1 | 1 (-0.24958) | -1 | -1 |
| G: -6257.50192 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.04441 HOMO: -6.50080 LUMO: 1.87759 factor:1 | 1 (-0.17679) | -1 | -1 |
| G: -6257.50192 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.98501 HOMO: -6.85727 LUMO: 1.99187 factor:1 | 1 (-0.11739) | -1 | -1 |
| G: -6257.50192 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.96228 HOMO: -6.58788 LUMO: 1.79051 factor:1 | 1 (-0.09467) | -1 | -1 |
| G: -6257.50192 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.95798 HOMO: -6.64230 LUMO: 2.16058 factor:1 | 1 (-0.09037) | -1 | -1 |
| G: -6257.50192 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.77390 HOMO: -6.58788 LUMO: 2.10616 factor:1 | -1 (0.09372) | -1 | -1 |
| G: -6257.50192 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.01303 HOMO: -7.01782 LUMO: 2.13609 factor:1 | 1 (-0.14542) | -1 | -1 |
| G: -6257.50192 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.99118 HOMO: -6.31304 LUMO: 2.31841 factor:1 | 1 (-0.12357) | -1 | -1 |
| G: -6257.50192 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.72486 HOMO: -6.94979 LUMO: 2.07895 factor:1 | -1 (0.14275) | -1 | -1 |
| G: -6257.50192 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.79600 HOMO: -6.88992 LUMO: 2.28031 factor:1 | -1 (0.07162) | -1 | -1 |
| G: -6257.50192 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.16248 HOMO: -6.66407 LUMO: 2.07623 factor:1 | 1 (-0.29486) | -1 | -1 |
| G: -6257.50192 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.05085 HOMO: -6.52529 LUMO: 1.70071 factor:1 | 1 (-1.18323) | -1 | -1 |
| G: -6257.50192 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.58670 HOMO: -6.58788 LUMO: 1.57282 factor:1 | 1 (-1.71908) | -1 | -1 |
| G: -6257.50192 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.88254 HOMO: -6.55250 LUMO: 1.95378 factor:1 | 1 (-2.01492) | -1 | -1 |
| G: -6257.50192 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.42392 HOMO: -6.24773 LUMO: 1.77962 factor:1 | 1 (-1.55630) | -1 | -1 |
| G: -6257.50192 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.31314 HOMO: -6.31304 LUMO: 2.18507 factor:1 | 1 (-1.44552) | -1 | -1 |
| G: -6257.50192 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.65973 HOMO: -6.18243 LUMO: 2.01636 factor:1 | 1 (-1.79211) | -1 | -1 |
| G: -6257.50192 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.68512 HOMO: -6.99877 LUMO: 2.14970 factor:1 | 1 (-1.81750) | -1 | -1 |
| G: -6257.50192 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.68901 HOMO: -6.72665 LUMO: 2.07079 factor:1 | 1 (-1.82139) | -1 | -1 |
| G: -6257.50192 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.00448 HOMO: -6.36202 LUMO: 2.17419 factor:1 | 1 (-1.13686) | -1 | -1 |
| G: -6257.50192 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.97814 HOMO: -6.78652 LUMO: 2.05718 factor:1 | 1 (-1.11052) | -1 | -1 |
| G: -6257.50192 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.96403 HOMO: -6.87360 LUMO: 2.34290 factor:1 | 1 (-0.09641) | -1 | -1 |
| G: -6257.50192 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.91355 HOMO: -6.62053 LUMO: 1.89391 factor:1 | 1 (-0.04593) | -1 | -1 |
| G: -6257.50192 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.04811 HOMO: -6.58788 LUMO: 1.83133 factor:1 | 1 (-0.18049) | -1 | -1 |
| G: -6257.50192 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.06512 HOMO: -7.08584 LUMO: 1.91568 factor:1 | 1 (-0.19750) | 1 | 1 |
| G: -6257.50192 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.83678 HOMO: -6.56883 LUMO: 1.81228 factor:1 | 1 (-0.96916) | -1 | -1 |
| G: -6257.50192 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.62485 HOMO: -6.66135 LUMO: 1.92384 factor:1 | 1 (-0.75724) | -1 | -1 |
| G: -6257.50192 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.91931 HOMO: -6.64502 LUMO: 2.15786 factor:1 | 1 (-1.05169) | -1 | -1 |
| G: -6257.50192 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.87104 HOMO: -6.71305 LUMO: 1.91840 factor:1 | 1 (-1.00342) | -1 | -1 |
| G: -6257.50192 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.83743 HOMO: -6.44094 LUMO: 1.74425 factor:1 | 1 (-0.96981) | -1 | -1 |
| G: -6257.50192 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.89446 HOMO: -6.51985 LUMO: 1.84221 factor:1 | 1 (-1.02685) | -1 | -1 |
| G: -6257.50192 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.90381 HOMO: -6.63414 LUMO: -0.24762 factor:1 | 1 (-0.03619) | -1 | -1 |
| G: -6257.50192 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.64742 HOMO: -6.60420 LUMO: -0.22585 factor:1 | -1 (0.22019) | -1 | -1 |
| G: -6257.50192 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.75458 HOMO: -7.19741 LUMO: 0.58232 factor:1 | -1 (0.11304) | -1 | -1 |
| G: -6257.50192 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.92993 HOMO: -6.77019 LUMO: -0.56872 factor:1 | 1 (-0.06231) | -1 | -1 |
| G: -6257.50192 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.65448 HOMO: -7.46136 LUMO: 0.28844 factor:1 | 1 (-1.78686) | -1 | -1 |
| G: -6257.50192 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.20467 HOMO: -6.60420 LUMO: -0.54151 factor:1 | 1 (-1.33706) | -1 | -1 |
| G: -6257.50192 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.76409 HOMO: -6.53890 LUMO: -0.46531 factor:1 | 1 (-0.89648) | -1 | -1 |
| G: -6257.50192 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.47325 HOMO: -6.81645 LUMO: -0.57144 factor:1 | 1 (-1.60564) | -1 | -1 |
| G: -6257.50192 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.72151 HOMO: -7.48041 LUMO: 0.28572 factor:1 | 1 (-0.85389) | -1 | -1 |
| G: -6257.50192 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.05779 HOMO: -6.75659 LUMO: -0.45715 factor:1 | 1 (-1.19017) | -1 | -1 |
| G: -6257.50192 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.51562 HOMO: -6.66135 LUMO: -0.41906 factor:1 | 1 (-1.64800) | -1 | -1 |
| G: -6257.50192 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.14318 HOMO: -6.55794 LUMO: -0.27483 factor:1 | 1 (-1.27556) | -1 | -1 |
| G: -6257.50192 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.15948 HOMO: -7.07496 LUMO: -0.63403 factor:1 | 1 (-1.29186) | -1 | -1 |
| G: -6257.50192 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.88807 HOMO: -7.12394 LUMO: 0.53334 factor:1 | 1 (-1.02045) | -1 | -1 |
| G: -6257.50192 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.89075 HOMO: -6.53617 LUMO: -0.25579 factor:1 | 1 (-0.02313) | -1 | -1 |
| G: -6257.50192 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.53028 HOMO: -6.50896 LUMO: -0.25034 factor:1 | -1 (0.33734) | -1 | -1 |
| G: -6257.50192 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.44627 HOMO: -7.17564 LUMO: -0.68573 factor:1 | -1 (0.42134) | -1 | -1 |
| G: -6257.50192 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.15560 HOMO: -6.53617 LUMO: -0.30749 factor:1 | -1 (0.71201) | -1 | -1 |
| G: -6257.50192 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.33542 HOMO: -6.55522 LUMO: -0.30749 factor:1 | -1 (0.53220) | -1 | -1 |
| G: -6257.50192 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.44355 HOMO: -7.05591 LUMO: -0.71022 factor:1 | -1 (0.42406) | -1 | -1 |
| G: -6257.50192 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.52435 HOMO: -7.17564 LUMO: -0.69933 factor:1 | 1 (-1.65674) | -1 | -1 |
| G: -6257.50192 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.66604 HOMO: -6.78380 LUMO: -0.67756 factor:1 | 1 (-1.79843) | -1 | -1 |
| G: -6257.50192 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12524.00349 HOMO: -6.62325 LUMO: 2.02725 factor:1 | 1 (-2.13588) | -1 | -1 |
| G: -6257.50192 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.37047 HOMO: -6.63414 LUMO: 1.91296 factor:1 | 1 (-1.50286) | -1 | -1 |
| G: -6257.50192 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.63285 HOMO: -6.83278 LUMO: 1.65717 factor:1 | 1 (-1.76523) | -1 | -1 |
| G: -6257.50192 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.95051 HOMO: -6.66407 LUMO: 1.95650 factor:1 | 1 (-2.08290) | -1 | -1 |
| G: -6257.50192 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.65374 HOMO: -6.61237 LUMO: 2.11432 factor:1 | 1 (-1.78613) | -1 | -1 |
| G: -6257.50192 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.90352 HOMO: -6.62053 LUMO: 2.09256 factor:1 | 1 (-2.03590) | -1 | -1 |
| G: -6257.50192 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12524.26777 HOMO: -6.78652 LUMO: 2.13609 factor:1 | 1 (-2.40015) | -1 | -1 |
| G: -6257.50192 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.39320 HOMO: -6.94707 LUMO: 1.81772 factor:1 | 1 (-0.52559) | -1 | -1 |
| G: -6257.50192 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.47008 HOMO: -6.85183 LUMO: 2.12793 factor:1 | 1 (-0.60246) | -1 | -1 |
| G: -6257.50192 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.97289 HOMO: -6.81101 LUMO: 1.83949 factor:1 | 1 (-1.10527) | -1 | -1 |
| G: -6257.50192 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.05621 HOMO: -6.98788 LUMO: 2.16058 factor:1 | 1 (-1.18859) | -1 | -1 |
| G: -6257.50192 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.49350 HOMO: -6.62869 LUMO: 2.00820 factor:1 | 1 (-0.62589) | -1 | -1 |
| G: -6257.50192 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.36498 HOMO: -6.34025 LUMO: 2.25855 factor:1 | 1 (-1.49736) | -1 | -1 |
| G: -6257.50192 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.99974 HOMO: -6.01372 LUMO: 2.01636 factor:1 | 1 (-2.13212) | -1 | -1 |
| G: -6257.50192 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.51437 HOMO: -6.89264 LUMO: 2.27487 factor:1 | 1 (-1.64675) | -1 | -1 |
| G: -6257.50192 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.95623 HOMO: -6.53073 LUMO: 2.20684 factor:1 | 1 (-2.08861) | -1 | -1 |
| G: -6257.50192 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.62224 HOMO: -6.83278 LUMO: 1.53744 factor:1 | 1 (-0.75463) | -1 | -1 |
| G: -6257.50192 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.45437 HOMO: -6.41917 LUMO: 1.82316 factor:1 | 1 (-0.58676) | -1 | -1 |
| G: -6257.50192 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.46627 HOMO: -6.56339 LUMO: 1.63813 factor:1 | 1 (-0.59865) | -1 | -1 |
| G: -6257.50192 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.74042 HOMO: -6.88992 LUMO: 1.65173 factor:1 | 1 (-0.87281) | -1 | -1 |
| G: -6257.50192 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.26157 HOMO: -6.63141 LUMO: 1.92112 factor:1 | 1 (-1.39396) | -1 | -1 |
| G: -6257.50192 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.18614 HOMO: -6.83822 LUMO: 1.88847 factor:1 | 1 (-1.31853) | -1 | -1 |
| G: -6257.50192 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.17474 HOMO: -6.84638 LUMO: 1.90480 factor:1 | 1 (-1.30713) | -1 | -1 |
| G: -6257.50192 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.58066 HOMO: -6.82462 LUMO: 1.70888 factor:1 | 1 (-0.71305) | -1 | -1 |
| G: -6257.50192 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.31892 HOMO: -6.82734 LUMO: 2.12521 factor:1 | 1 (-0.45130) | -1 | -1 |
| G: -6257.50192 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.46289 HOMO: -6.94435 LUMO: 1.87214 factor:1 | 1 (-0.59528) | -1 | -1 |
| G: -6257.50192 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.05972 HOMO: -6.98516 LUMO: 2.51433 factor:1 | 1 (-1.19210) | -1 | -1 |
| G: -6257.50192 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.94108 HOMO: -6.74026 LUMO: 2.15514 factor:1 | 1 (-1.07346) | -1 | -1 |
| G: -6257.50192 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.19684 HOMO: -6.93618 LUMO: 2.54426 factor:1 | 1 (-1.32922) | -1 | -1 |
| G: -6257.50192 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.65122 HOMO: -6.28583 LUMO: 2.53610 factor:1 | 1 (-0.78361) | -1 | -1 |
| G: -6257.50192 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.48335 HOMO: -6.56883 LUMO: 1.94834 factor:1 | 1 (-0.61574) | -1 | -1 |
| G: -6257.50192 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.27826 HOMO: -7.08584 LUMO: 1.99187 factor:1 | 1 (-0.41065) | 1 | 1 |
| G: -6257.50192 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.01139 HOMO: -6.19059 LUMO: 1.99732 factor:1 | 1 (-1.14378) | -1 | -1 |
| G: -6257.50192 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.79931 HOMO: -6.78108 LUMO: 2.03813 factor:1 | 1 (-0.93169) | -1 | -1 |
| G: -6257.50192 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.12465 HOMO: -6.82189 LUMO: 1.77418 factor:1 | 1 (-1.25703) | -1 | -1 |
| G: -6257.50192 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.29190 HOMO: -6.45454 LUMO: 1.78779 factor:1 | 1 (-0.42428) | -1 | -1 |
| G: -6257.50192 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.54137 HOMO: -6.84366 LUMO: 1.77690 factor:1 | 1 (-0.67375) | -1 | -1 |
| G: -6257.50192 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.70067 HOMO: -6.74026 LUMO: 1.67622 factor:1 | 1 (-0.83305) | -1 | -1 |
| G: -6257.50192 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.72303 HOMO: -6.76475 LUMO: 2.40277 factor:1 | 1 (-0.85542) | -1 | -1 |
| G: -6257.50192 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.23194 HOMO: -6.65863 LUMO: 1.86670 factor:1 | 1 (-1.36432) | -1 | -1 |
| G: -6257.50192 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.61699 HOMO: -6.50080 LUMO: 1.93201 factor:1 | 1 (-0.74937) | -1 | -1 |
| G: -6257.50192 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.10606 HOMO: -6.34842 LUMO: 1.70888 factor:1 | 1 (-1.23844) | -1 | -1 |
| G: -6257.50192 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.22174 HOMO: -6.60692 LUMO: 2.20140 factor:1 | 1 (-1.35412) | -1 | -1 |
| G: -6257.50192 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.65519 HOMO: -6.74026 LUMO: 2.14970 factor:1 | 1 (-0.78758) | -1 | -1 |
| G: -6257.50192 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.65386 HOMO: -6.63686 LUMO: 2.17419 factor:1 | 1 (-0.78625) | -1 | -1 |
| G: -6257.50192 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.74317 HOMO: -6.81917 LUMO: 2.10072 factor:1 | 1 (-0.87555) | -1 | -1 |
| G: -6257.50192 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.26386 HOMO: -6.92802 LUMO: 2.04358 factor:1 | 1 (-1.39624) | -1 | -1 |
| G: -6257.50192 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.22043 HOMO: -6.56067 LUMO: -0.47620 factor:1 | 1 (-1.35281) | -1 | -1 |
| G: -6257.50192 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.33443 HOMO: -6.56611 LUMO: -0.77008 factor:1 | 1 (-0.46681) | -1 | -1 |
| G: -6257.50192 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.48512 HOMO: -6.78380 LUMO: -0.64763 factor:1 | 1 (-0.61751) | -1 | -1 |
| G: -6257.50192 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.54994 HOMO: -6.51985 LUMO: -0.24490 factor:1 | 1 (-0.68233) | -1 | -1 |
| G: -6257.50192 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.24715 HOMO: -6.52529 LUMO: -0.27483 factor:1 | 1 (-1.37954) | -1 | -1 |
| G: -6257.50192 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.07654 HOMO: -7.10489 LUMO: -0.62586 factor:1 | 1 (-1.20892) | -1 | -1 |
| G: -6257.50192 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.92540 HOMO: -7.18108 LUMO: 0.48980 factor:1 | 1 (-1.05779) | -1 | -1 |
| G: -6257.50192 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.67819 HOMO: -7.14299 LUMO: -0.63947 factor:1 | 1 (-0.81057) | -1 | -1 |
| G: -6257.50192 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.02285 HOMO: -6.70761 LUMO: -0.54423 factor:1 | 1 (-1.15523) | -1 | -1 |
| G: -6257.50192 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.11256 HOMO: -7.32258 LUMO: -1.03675 factor:1 | 1 (-1.24495) | -1 | -1 |
| G: -6257.50192 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.64286 HOMO: -6.65046 LUMO: -0.41361 factor:1 | 1 (-1.77524) | -1 | -1 |
| G: -6257.50192 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.62762 HOMO: -6.76475 LUMO: -0.60137 factor:1 | 1 (-1.76001) | -1 | -1 |
| G: -6257.50192 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.05558 HOMO: -6.77836 LUMO: -0.54423 factor:1 | 1 (-1.18797) | -1 | -1 |
| G: -6257.50192 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.07869 HOMO: -7.52395 LUMO: 0.26395 factor:1 | 1 (-1.21107) | -1 | -1 |
| G: -6257.50192 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.52033 HOMO: -6.93890 LUMO: -0.72382 factor:1 | 1 (-1.65271) | -1 | -1 |
| G: -6257.50192 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12524.19005 HOMO: -6.72938 LUMO: -0.47348 factor:1 | 1 (-2.32244) | -1 | -1 |
| G: -6257.50192 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.48707 HOMO: -6.66951 LUMO: -0.40817 factor:1 | 1 (-1.61946) | -1 | -1 |
| G: -6257.50192 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.56308 HOMO: -6.60420 LUMO: -0.19320 factor:1 | 1 (-1.69546) | -1 | -1 |
| G: -6257.50192 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12524.17185 HOMO: -6.67495 LUMO: -0.27211 factor:1 | 1 (-2.30423) | -1 | -1 |
| G: -6257.50192 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12524.04918 HOMO: -7.23823 LUMO: -0.62858 factor:1 | 1 (-2.18156) | -1 | -1 |
| G: -6257.50192 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.55900 HOMO: -7.27088 LUMO: 0.53334 factor:1 | 1 (-0.69139) | -1 | -1 |
| G: -6257.50192 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.13197 HOMO: -7.20013 LUMO: 0.59049 factor:1 | 1 (-1.26435) | -1 | -1 |
| G: -6257.50192 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.10470 HOMO: -6.60148 LUMO: -0.20953 factor:1 | 1 (-1.23708) | -1 | -1 |
| G: -6257.50192 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.06100 HOMO: -6.69400 LUMO: -0.51974 factor:1 | 1 (-1.19338) | -1 | -1 |
| G: -6257.50192 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.50991 HOMO: -7.40422 LUMO: -0.98777 factor:1 | 1 (-0.64230) | -1 | -1 |
| G: -6257.50192 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.07139 HOMO: -6.88176 LUMO: -0.71022 factor:1 | 1 (-1.20378) | -1 | -1 |
| G: -6257.50192 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.54172 HOMO: -6.86271 LUMO: -0.59321 factor:1 | 1 (-0.67411) | -1 | -1 |
| G: -6257.50192 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.04960 HOMO: -6.73754 LUMO: -0.55239 factor:1 | 1 (-1.18198) | -1 | -1 |
| G: -6257.50192 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.86369 HOMO: -6.71033 LUMO: 1.57010 factor:1 | 1 (-0.99607) | -1 | -1 |
| G: -6257.50192 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.11648 HOMO: -6.69672 LUMO: 1.68711 factor:1 | 1 (-1.24887) | -1 | -1 |
| G: -6257.50192 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.45508 HOMO: -6.67495 LUMO: 2.03813 factor:1 | 1 (-0.58747) | -1 | -1 |
| G: -6257.50192 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.08380 HOMO: -6.54434 LUMO: 1.83677 factor:1 | 1 (-1.21619) | -1 | -1 |
| G: -6257.50192 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.02679 HOMO: -6.57155 LUMO: 1.77146 factor:1 | 1 (-1.15918) | -1 | -1 |
| G: -6257.50192 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.92627 HOMO: -6.76747 LUMO: 1.87759 factor:1 | 1 (-1.05866) | -1 | -1 |
| G: -6257.50192 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.47625 HOMO: -6.58243 LUMO: 1.61364 factor:1 | 1 (-0.60864) | -1 | -1 |
| G: -6257.50192 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.35143 HOMO: -6.61781 LUMO: 2.13881 factor:1 | 1 (-0.48382) | -1 | -1 |
| G: -6257.50192 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.21042 HOMO: -6.62597 LUMO: 2.00276 factor:1 | 1 (-1.34280) | -1 | -1 |
| G: -6257.50192 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.57801 HOMO: -7.01237 LUMO: 1.95922 factor:1 | 1 (-1.71040) | -1 | -1 |
| G: -6257.50192 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12524.37974 HOMO: -7.03959 LUMO: 2.16875 factor:1 | 1 (-2.51213) | -1 | -1 |
| G: -6257.50192 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12524.37958 HOMO: -6.83278 LUMO: 1.91296 factor:1 | 1 (-2.51196) | -1 | -1 |
| G: -6257.50192 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12524.38793 HOMO: -6.40012 LUMO: 1.95650 factor:1 | 1 (-2.52032) | -1 | -1 |
| G: -6257.50192 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.06073 HOMO: -6.50080 LUMO: 1.73337 factor:1 | 1 (-1.19311) | -1 | -1 |
| G: -6257.50192 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.99844 HOMO: -6.95795 LUMO: 2.28848 factor:1 | 1 (-1.13082) | -1 | -1 |
| G: -6257.50192 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.65506 HOMO: -6.63686 LUMO: 2.20140 factor:1 | 1 (-0.78744) | -1 | -1 |
| G: -6257.50192 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.44858 HOMO: -6.57427 LUMO: 1.87214 factor:1 | 1 (-0.58096) | -1 | -1 |
| G: -6257.50192 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.17725 HOMO: -6.38379 LUMO: 2.32113 factor:1 | 1 (-0.30964) | -1 | -1 |
| G: -6257.50192 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.06894 HOMO: -6.63958 LUMO: 2.04902 factor:1 | 1 (-1.20133) | -1 | -1 |
| G: -6257.50192 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.99446 HOMO: -6.70216 LUMO: 1.93201 factor:1 | 1 (-2.12684) | -1 | -1 |
| G: -6257.50192 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.04992 HOMO: -6.80557 LUMO: 2.23678 factor:1 | 1 (-1.18231) | -1 | -1 |
| G: -6257.50192 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12524.06962 HOMO: -6.72938 LUMO: 2.28304 factor:1 | 1 (-2.20200) | -1 | -1 |
| G: -6257.50192 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.98480 HOMO: -6.56067 LUMO: 1.66806 factor:1 | 1 (-2.11718) | -1 | -1 |
| G: -6257.50192 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.42789 HOMO: -6.95523 LUMO: 2.33474 factor:1 | 1 (-1.56027) | -1 | -1 |
| G: -6257.50192 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.68814 HOMO: -6.59876 LUMO: 2.30480 factor:1 | 1 (-1.82052) | -1 | -1 |
| G: -6257.50192 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.34713 HOMO: -6.87360 LUMO: 1.75786 factor:1 | 1 (-1.47951) | -1 | -1 |
| G: -6257.50192 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.42472 HOMO: -7.06408 LUMO: 1.99187 factor:1 | -1 (0.44289) | 1 | 1 |
| G: -6257.50192 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.03771 HOMO: -6.95795 LUMO: 1.88847 factor:1 | 1 (-1.17009) | -1 | -1 |
| G: -6257.50192 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.13088 HOMO: -6.85455 LUMO: 1.63813 factor:1 | 1 (-1.26326) | -1 | -1 |
| G: -6257.50192 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.81523 HOMO: -7.09129 LUMO: 2.31569 factor:1 | 1 (-0.94761) | 1 | 1 |
| G: -6257.50192 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.32801 HOMO: -6.91441 LUMO: 1.68983 factor:1 | -1 (0.53960) | -1 | -1 |
| G: -6257.50192 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.29926 HOMO: -6.89809 LUMO: 2.23678 factor:1 | 1 (-1.43165) | -1 | -1 |
| G: -6257.50192 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.39894 HOMO: -6.78652 LUMO: 1.98371 factor:1 | 1 (-1.53132) | -1 | -1 |
| G: -6257.50192 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.07025 HOMO: -6.94707 LUMO: 2.23678 factor:1 | 1 (-1.20263) | -1 | -1 |
| G: -6257.50192 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.94582 HOMO: -7.07224 LUMO: 2.13337 factor:1 | 1 (-0.07821) | 1 | 1 |
| G: -6257.50192 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.06520 HOMO: -6.94979 LUMO: 2.28031 factor:1 | 1 (-0.19758) | -1 | -1 |
| G: -6257.50192 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.74008 HOMO: -6.60965 LUMO: 2.20412 factor:1 | -1 (0.12754) | -1 | -1 |
| G: -6257.50192 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.30678 HOMO: -6.87360 LUMO: 2.40277 factor:1 | 1 (-0.43916) | -1 | -1 |
| G: -6257.50192 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.67126 HOMO: -6.92802 LUMO: 1.89663 factor:1 | -1 (0.19636) | -1 | -1 |
| G: -6257.50192 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.35280 HOMO: -6.88448 LUMO: 2.02725 factor:1 | -1 (0.51481) | -1 | -1 |
| G: -6257.50192 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.05504 HOMO: -6.69128 LUMO: 1.55105 factor:1 | 1 (-1.18742) | -1 | -1 |
| G: -6257.50192 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.61053 HOMO: -6.54978 LUMO: 1.93201 factor:1 | 1 (-1.74292) | -1 | -1 |
| G: -6257.50192 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.10748 HOMO: -6.19331 LUMO: 1.46941 factor:1 | 1 (-1.23986) | -1 | -1 |
| G: -6257.50192 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.76423 HOMO: -6.55794 LUMO: 1.89663 factor:1 | 1 (-0.89662) | -1 | -1 |
| G: -6257.50192 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.55330 HOMO: -6.07630 LUMO: 1.94289 factor:1 | -1 (0.31432) | -1 | -1 |
| G: -6257.50192 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.49230 HOMO: -7.46408 LUMO: 0.31565 factor:1 | 1 (-1.62468) | -1 | -1 |
| G: -6257.50192 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.65282 HOMO: -6.63958 LUMO: -0.61770 factor:1 | 1 (-1.78520) | -1 | -1 |
| G: -6257.50192 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.24244 HOMO: -6.81101 LUMO: -0.57960 factor:1 | 1 (-1.37483) | -1 | -1 |
| G: -6257.50192 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.15268 HOMO: -6.74298 LUMO: -0.57960 factor:1 | 1 (-0.28507) | -1 | -1 |
| G: -6257.50192 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.35293 HOMO: -6.63686 LUMO: -0.42994 factor:1 | 1 (-0.48532) | -1 | -1 |
| G: -6257.50192 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.98397 HOMO: -6.60965 LUMO: -0.41089 factor:1 | 1 (-0.11636) | -1 | -1 |
| G: -6257.50192 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.68306 HOMO: -6.60692 LUMO: -0.80274 factor:1 | 1 (-0.81544) | -1 | -1 |
| G: -6257.50192 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.25768 HOMO: -6.58788 LUMO: -0.78097 factor:1 | 1 (-1.39007) | -1 | -1 |
| G: -6257.50192 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.45499 HOMO: -6.67767 LUMO: -0.48436 factor:1 | 1 (-1.58738) | -1 | -1 |
| G: -6257.50192 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.08448 HOMO: -6.63141 LUMO: -0.40545 factor:1 | 1 (-1.21687) | -1 | -1 |
| G: -6257.50192 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.16880 HOMO: -6.62053 LUMO: -0.83811 factor:1 | -1 (0.69882) | -1 | -1 |
| G: -6257.50192 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.62416 HOMO: -6.59604 LUMO: -0.35375 factor:1 | -1 (0.24346) | -1 | -1 |
| G: -6257.50192 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.45003 HOMO: -6.34297 LUMO: -0.39729 factor:1 | -1 (0.41759) | -1 | -1 |
| G: -6257.50192 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.85411 HOMO: -6.67223 LUMO: 1.97827 factor:1 | 1 (-0.98649) | -1 | -1 |
| G: -6257.50192 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.07681 HOMO: -6.40012 LUMO: 1.89935 factor:1 | 1 (-1.20919) | -1 | -1 |
| G: -6257.50192 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.81631 HOMO: -6.74842 LUMO: 1.97283 factor:1 | 1 (-0.94870) | -1 | -1 |
| G: -6257.50192 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.03663 HOMO: -6.76747 LUMO: 2.17147 factor:1 | -1 (0.83098) | -1 | -1 |
| G: -6257.50192 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.19500 HOMO: -6.72121 LUMO: 1.55649 factor:1 | -1 (0.67261) | -1 | -1 |
| G: -6257.50192 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.11238 HOMO: -6.97700 LUMO: 2.04085 factor:1 | 1 (-0.24477) | -1 | -1 |
| G: -6257.50192 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.29979 HOMO: -7.06680 LUMO: 2.04085 factor:1 | 1 (-0.43217) | 1 | 1 |
| G: -6257.50192 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.93028 HOMO: -7.09673 LUMO: 2.35106 factor:1 | 1 (-0.06267) | 1 | 1 |
| G: -6257.50192 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.42235 HOMO: -6.83006 LUMO: 2.14970 factor:1 | 1 (-0.55473) | -1 | -1 |
| G: -6257.50192 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12520.46637 HOMO: -6.72665 LUMO: 2.20140 factor:1 | -1 (1.40125) | -1 | -1 |
| G: -6257.50192 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.05767 HOMO: -6.77291 LUMO: 2.34562 factor:1 | -1 (0.80995) | -1 | -1 |
| G: -6257.50192 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12520.91318 HOMO: -6.73754 LUMO: 2.00276 factor:1 | -1 (0.95444) | -1 | -1 |
| G: -6257.50192 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.23150 HOMO: -7.04231 LUMO: 1.92112 factor:1 | -1 (0.63612) | -1 | -1 |
| G: -6257.50192 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.30673 HOMO: -6.83822 LUMO: 1.72248 factor:1 | 1 (-0.43911) | -1 | -1 |
| G: -6257.50192 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12520.14056 HOMO: -6.57971 LUMO: 2.16603 factor:1 | -1 (1.72705) | -1 | -1 |
| G: -6257.50192 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12520.90485 HOMO: -6.80013 LUMO: 1.88575 factor:1 | -1 (0.96277) | -1 | -1 |
| G: -6257.50192 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.37099 HOMO: -6.93618 LUMO: 2.18235 factor:1 | 1 (-1.50337) | -1 | -1 |
| G: -6257.50192 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.54522 HOMO: -6.54706 LUMO: 1.91024 factor:1 | 1 (-1.67761) | -1 | -1 |
| G: -6257.50192 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.20625 HOMO: -7.06952 LUMO: 2.18507 factor:1 | 1 (-1.33864) | 1 | 1 |
| G: -6257.50192 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.59751 HOMO: -7.05047 LUMO: 1.82044 factor:1 | 1 (-0.72989) | -1 | -1 |
| G: -6257.50192 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.01099 HOMO: -6.87632 LUMO: 1.92657 factor:1 | 1 (-0.14338) | -1 | -1 |
| G: -6257.50192 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.14792 HOMO: -6.58788 LUMO: 1.91568 factor:1 | 1 (-0.28030) | -1 | -1 |
| G: -6257.50192 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.86274 HOMO: -7.17292 LUMO: 1.90752 factor:1 | -1 (0.00487) | 1 | 1 |
| G: -6257.50192 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.25772 HOMO: -6.93890 LUMO: 1.80684 factor:1 | 1 (-0.39010) | -1 | -1 |
| G: -6257.50192 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.03201 HOMO: -7.10761 LUMO: 2.20956 factor:1 | -1 (0.83561) | 1 | 1 |
| G: -6257.50192 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12520.97563 HOMO: -6.85727 LUMO: 2.13609 factor:1 | -1 (0.89199) | -1 | -1 |
| G: -6257.50192 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.22633 HOMO: -6.64502 LUMO: 1.38506 factor:1 | 1 (-1.35872) | -1 | -1 |
| G: -6257.50192 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.33554 HOMO: -6.87360 LUMO: 1.15648 factor:1 | 1 (-0.46793) | -1 | -1 |
| G: -6257.50192 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.39992 HOMO: -6.67223 LUMO: 2.07351 factor:1 | 1 (-1.53230) | -1 | -1 |
| G: -6257.50192 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.46159 HOMO: -6.29671 LUMO: 2.43270 factor:1 | 1 (-0.59397) | -1 | -1 |
| G: -6257.50192 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.10089 HOMO: -6.90897 LUMO: 2.28848 factor:1 | 1 (-1.23327) | -1 | -1 |
| G: -6257.50192 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.18751 HOMO: -7.04231 LUMO: 1.70071 factor:1 | 1 (-0.31990) | -1 | -1 |
| G: -6257.50192 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.64349 HOMO: -6.69944 LUMO: 1.94834 factor:1 | 1 (-0.77588) | -1 | -1 |
| G: -6257.50192 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.34156 HOMO: -6.56067 LUMO: 2.20956 factor:1 | 1 (-0.47394) | -1 | -1 |
| G: -6257.50192 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.10810 HOMO: -6.65046 LUMO: 2.06807 factor:1 | 1 (-1.24049) | -1 | -1 |
| G: -6257.50192 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.87647 HOMO: -7.08584 LUMO: 1.98915 factor:1 | 1 (-2.00885) | 1 | 1 |
| G: -6257.50192 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.23091 HOMO: -6.69400 LUMO: 2.09256 factor:1 | 1 (-1.36329) | -1 | -1 |
| G: -6257.50192 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.97920 HOMO: -6.62869 LUMO: 2.16331 factor:1 | 1 (-1.11159) | -1 | -1 |
| G: -6257.50192 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.20281 HOMO: -6.85183 LUMO: 2.16058 factor:1 | -1 (0.66480) | -1 | -1 |
| G: -6257.50192 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.03672 HOMO: -6.54706 LUMO: 1.92384 factor:1 | -1 (0.83090) | -1 | -1 |
| G: -6257.50192 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.34833 HOMO: -6.84366 LUMO: 2.48984 factor:1 | 1 (-0.48072) | -1 | -1 |
| G: -6257.50192 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.00824 HOMO: -6.77291 LUMO: 2.46263 factor:1 | 1 (-0.14063) | -1 | -1 |
| G: -6257.50192 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12520.72349 HOMO: -7.01782 LUMO: 2.31025 factor:1 | -1 (1.14413) | -1 | -1 |
| G: -6257.50192 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12520.86183 HOMO: -6.94707 LUMO: 2.29664 factor:1 | -1 (1.00579) | -1 | -1 |
| G: -6257.50192 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.33374 HOMO: -6.64230 LUMO: 1.97283 factor:1 | 1 (-1.46612) | -1 | -1 |
| G: -6257.50192 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.07267 HOMO: -6.47359 LUMO: 2.20412 factor:1 | 1 (-1.20506) | -1 | -1 |
| G: -6257.50192 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.37036 HOMO: -6.90625 LUMO: 1.92384 factor:1 | 1 (-1.50275) | -1 | -1 |
| G: -6257.50192 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.91688 HOMO: -7.17020 LUMO: 2.06807 factor:1 | 1 (-2.04926) | 1 | 1 |
| G: -6257.50192 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.89904 HOMO: -6.65046 LUMO: 2.20956 factor:1 | 1 (-1.03142) | -1 | -1 |
| G: -6257.50192 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.13499 HOMO: -7.07496 LUMO: 1.82861 factor:1 | 1 (-1.26737) | 1 | 1 |
| G: -6257.50192 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.73158 HOMO: -6.83006 LUMO: 2.14970 factor:1 | 1 (-0.86396) | -1 | -1 |
| G: -6257.50192 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.10204 HOMO: -6.92802 LUMO: 1.99187 factor:1 | 1 (-0.23443) | -1 | -1 |
| G: -6257.50192 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.88212 HOMO: -6.69672 LUMO: 2.36739 factor:1 | 1 (-0.01450) | -1 | -1 |
| G: -6257.50192 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.93741 HOMO: -7.13755 LUMO: 2.00276 factor:1 | 1 (-0.06980) | 1 | 1 |
| G: -6257.50192 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.20558 HOMO: -6.92530 LUMO: 2.25582 factor:1 | 1 (-0.33797) | -1 | -1 |
| G: -6257.50192 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.03282 HOMO: -6.77564 LUMO: 1.97827 factor:1 | 1 (-0.16520) | -1 | -1 |
| G: -6257.50192 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.77001 HOMO: -6.87904 LUMO: 1.60003 factor:1 | -1 (0.09761) | -1 | -1 |
| G: -6257.50192 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.80114 HOMO: -6.62869 LUMO: 1.90480 factor:1 | -1 (0.06648) | -1 | -1 |
| G: -6257.50192 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.12433 HOMO: -6.71033 LUMO: 1.54833 factor:1 | 1 (-0.25671) | -1 | -1 |
| G: -6257.50192 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.78881 HOMO: -6.74298 LUMO: 1.47486 factor:1 | -1 (0.07880) | -1 | -1 |
| G: -6257.50192 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.69504 HOMO: -6.77019 LUMO: 1.90480 factor:1 | -1 (0.17257) | -1 | -1 |
| G: -6257.50192 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.02789 HOMO: -6.70489 LUMO: 1.99459 factor:1 | 1 (-0.16028) | -1 | -1 |